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# Suppression of Mott–Hubbard states and metal-insulator transitions in the two band Hubbard model

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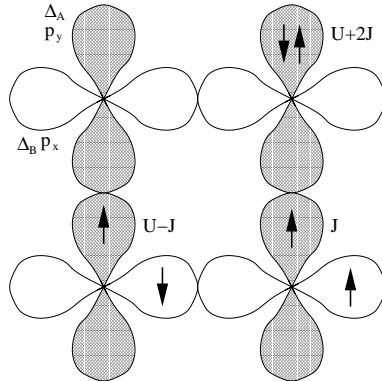
**Abstract.** I investigate band and Mott insulating states in a two-band Hubbard model, with the aim of understanding the differences between the idealised one-orbital model and the more realistic multi-band case. Using a projection ansatz I show that additional orbitals suppress the metal-insulator transition, leading to a critical coupling of approximately eight times the bare band-width. I also demonstrate the effects of orbital ordering, which hinder Mott-Hubbard states and open a band gap. Since multi-band correlations are common in real materials, this work suggests that the existence of very strongly correlated band insulators may be more common than Mott-Hubbard insulators. [PUBLISHED AS J.PHYS.:CONDENS. MATTER **17** 1385-1397 (2005)]

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## 1. Introduction

The prediction and experimental confirmation of a correlation driven Mott transition is one of the great success stories from the study of correlated electron systems. Mott postulated the existence of an insulating state, when the Coulomb repulsion is significantly larger than the kinetic energy, as the antithesis of the free-electron metal [1]. The simplest model of the Mott transition is the Hubbard model, where a one-band tight-binding model is supplemented with a site-local repulsion between electrons of opposite spin, which partially represents the Coulomb interaction [2]. The one-band Hubbard model is insulating at half-filling, provided that the interaction between electrons is significantly higher than the inter-site hopping, since electrons may not move freely without paying a large energy penalty.

The single-band Hubbard model is very effective for systems in which the electrons at the Fermi-energy are well separated from those in other bands. In many systems, including the much discussed cuprate superconductors, it is clear that two or even more bands are close in energy and inter-band coupling is expected to be relevant. In particular, electrons may favour configurations associated with Hund's rule coupling between orbitals. The aim of this paper is to understand the differences between one- and two-band Hubbard models, including the effects of realistic orbitals and orbital ordering. It is particularly important to classify this behaviour, since band-structure theories tend to play down the rôle of strong correlations, while many-body theorists are inclined to over-simplify their models.

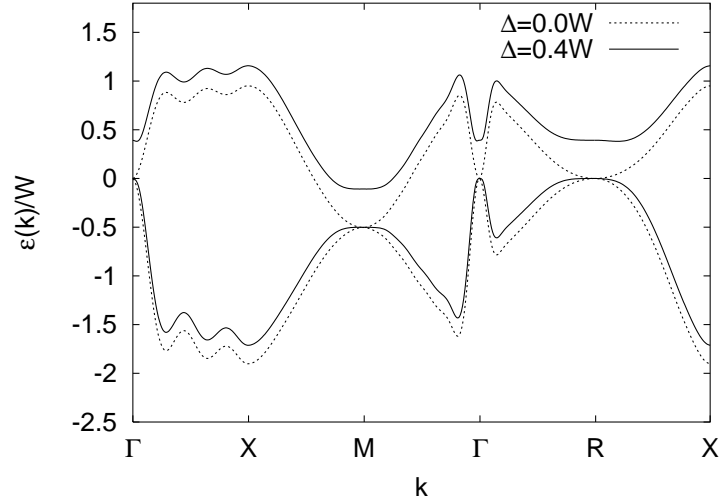


**Figure 1.** In the model used in this work, the first set of  $p$ -orbitals extend in the  $x$ -direction, while the second set extend in the  $y$ -direction. In addition to the orbitals, the energy levels of the orbitals represented by  $\Delta_i$  may be changed, adding a competing mechanism for an insulating state to the system. Electrons interact via a Coulomb repulsion, and inter-orbital spins interact via a Hund’s rule coupling,  $J$ . For two electrons of opposite spin in the same orbital, the repulsion is  $U + 2J$ , and for electrons in different orbitals, it is  $U - J$ .

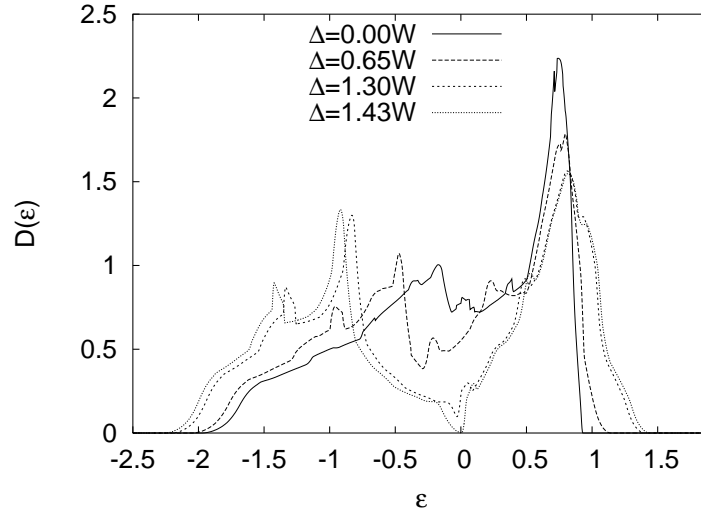
Orbital ordering and weak-correlation Hartree-Fock effects are the typical origins of band-gaps in electronic structure calculations. The name *band insulator* is given, because in the event of weak interactions, the gap separates *single-electron bands*. An alternative mechanism for the opening of band-gaps is found for very strong inter-electron coupling, where electron correlations drive an insulating state at half-filling (exactly two electrons per site in this paper). The origin of the strongly-interacting *Mott-Hubbard insulator* is far more complicated in origin, and the gap is formed by many-body interactions between electrons of the same type and may be found in systems with strong correlation. A full classification of different insulating states may be found e.g. in reference [3].

The treatment of excitations in the two-band Hubbard model presented here involves a local ansatz-based approach to the correlation problem. For the ground state, an approximation which treats local spin and density fluctuations is used. Such an approach has been applied to  $d$ -electrons in transition metals by Stollhoff *et al.* [4]. Excited states are also treated using a local spin and density fluctuation approximation using the approach of Becker *et al.* [5]. The present work modifies the method of Unger *et al.* [6], although in this paper we are interested in the physics of the two-band Hubbard model for a range of interactions, rather than the specific details of real metallic systems like Nickel.

This paper is organised as follows. The model is presented in section 2 along with a discussion of the non-interacting problem, and details of the metal to band insulator transition. In section 3, the effects of correlation on the orbitally degenerate model are calculated for a range of Coulomb and Hund’s coupling. In section 4, the effects of changing the orbital degeneracy on correlated states are discussed. Conclusions are presented in section 5. In particular, two-band effects have a dramatic influence on the Mott transition and change the critical coupling by an order of magnitude.



**Figure 2.** Non-interacting band structure resulting from diagonalisation of the canonical structure matrix. The orbitals are strongly hybridised and there are two clearly separated bands. There are several degenerate regions along the high symmetry directions. Also shown is the non-interacting band structure as the energy level of one of the orbitals is raised by  $0.4W$ . This removes the degeneracies at high-symmetry points. At a critical energy difference of  $\Delta = 1.43W$ , the bands split completely, and the system is driven through a metal-to-band insulator transition. It should be stressed that *band insulators* have very different properties to correlation driven *Mott insulators*, which are the main subject of this paper.



**Figure 3.** The bare density of states resulting from the canonical structure matrix. There is no particle-hole symmetry. Also shown is the effect of changing the relative energy levels of the orbitals. Precursors to the band are visible just below the Fermi energy. The opening of a band-insulating gap can be seen at  $\Delta = 1.43W$ .

## 2. Model and formalism

The model used in this work describes electrons on a simple cubic lattice of interlocking  $p$ -orbitals, and is shown schematically in figure 1. Two bands are considered, with one orbital aligned along the  $x$ -axis and the other along the  $y$ -axis. This model has the property that hopping within the plane is equivalent along both axes, with a different (smaller) hopping along the  $z$ -axis. As such, the model may be considered to describe a quasi-2D system. Electrons may be created in the  $m$ th band with the operator  $d_{m\mathbf{k}\sigma}^\dagger$ . Each band has a Coulomb repulsion,  $U$ , and spins from different bands interact with each other via a local coupling,  $J$ . The most general form of model for treating locally interacting electrons is,

$$\begin{aligned} H = & \sum_{m\mathbf{k}\sigma} (\epsilon_{m\mathbf{k}} + \epsilon_F) d_{m\mathbf{k}\sigma}^\dagger d_{m\mathbf{k}\sigma} \\ & + (U + 2J) \sum_{iI} n_{iI\uparrow} n_{iI\downarrow} + \frac{1}{2}(U - J) \sum_{I\sigma\sigma', i \neq j} n_{Ii\sigma} n_{Ij\sigma'} \\ & - J \sum_{I, i \neq j} \mathbf{s}_i \cdot \mathbf{s}_j \end{aligned} \quad (1)$$

The non-interacting (or bare) band structure is found by diagonalising the one-electron canonical structure matrix [7],

$$S_{l'm';lm}^{\mathbf{k}} = g_{l'm';lm} \Sigma_{\lambda,\mu}^{\mathbf{k}} \quad (2)$$

where

$$\Sigma_{\lambda,\mu}^{\mathbf{k}} = \sum_{R \neq 0} e^{i\mathbf{k} \cdot \mathbf{R}} \left( \frac{S}{R} \right)^{\lambda+1} [\sqrt{4\pi} i^\lambda Y_{\lambda\mu}(\hat{\mathbf{R}})]^* \quad (3)$$

and

$$\begin{aligned} g_{l'm';lm} = & 2(-1)^{m+1} \left( \frac{(2l'+1)(2l+1)}{(2\lambda+1)} \right)^{1/2} \\ & \times \left( \frac{(\lambda+\mu)!(\lambda-\mu)!}{(l'+m')!(l'-m')!(l+m)!(l-m)!} \right)^{1/2} \end{aligned} \quad (4)$$

$Y_{\lambda\mu}(\mathbf{R})$  are the spherical harmonics, and  $\lambda = l' + l$ ,  $\mu = m' - m$ . After diagonalisation, the Eigenvalues represent the dispersion of the non-interacting bands, and Eigenvectors transform the problem from the band to the orbital representation. The model represented by the canonical-structure matrix is more complicated than that typically used for Hubbard models, since hopping is allowed between all sites rather than just nearest neighbours. The largest contributions are expected from nearest and next-nearest neighbours, although other smaller corrections are expected from longer range hopping.

One may also augment the model by shifting the energies of individual orbitals,

$$H_0 \rightarrow H_0 + \sum_{Ii\sigma} \Delta_i n_{Ii\sigma} \quad (5)$$

resulting in an orbitally diagonal matrix that is simply added to the canonical structure matrix,

$$\Delta_{\lambda,\mu} = \Delta_\lambda \delta_{\lambda,\mu} \quad (6)$$

The resulting band structure for the two-band  $p$ -orbital model is shown in figure 2. As with all figures, the Fermi energy is at  $\epsilon = 0$ . For a model with degenerate orbital energies, the bands hybridise into upper and lower bands. There are several degenerate points along the high symmetry directions. Modifying the orbital energies has the effect of separating the upper and lower bands, creating local band gaps. It can be seen in the figure that the highest energies of the lowest band are higher than the lowest of the higher band, and there is no universal band gap. The band that is lower in energy is favoured by electrons. As  $\Delta$  is increased, the local band gaps become larger, until there is no overlap and the band gap is universal across the Brillouin zone. Then, a metal-to-band insulator transition takes place at half filling, since the ground state favours one completely filled and one empty band.

I turn to the evolution of the band insulating state in figure 3. The total DOS is calculated using the analytic tetrahedron method [8]. As  $\Delta$  is increased, the precursor of the band gap can be seen just below the Fermi energy at  $\epsilon = 0$ . The gap finally opens at  $\Delta = 1.43W$ , where the band width  $W = \sqrt{M_2 - M_1^2}$  is taken as the band width of the bare ( $\Delta = 0$ ) dispersion, and  $M_n$  is the  $n$ th moment of the DOS.

Such a band insulator is trivially formed, and effects of non-degenerate orbital energies are expected to be found in a wide range of materials. However, it is the effects of correlation that are the main subject of this paper. When one includes a simple Hubbard interaction in the lower band, it is clear that some electrons will be excluded from the lower orbital, and the band-insulating state will be destroyed. From the inverse viewpoint, the effects of correlation are hindered by a band state. In the remaining sections of this paper, I will investigate first correlations, and then the effects of band insulating states on these correlations.

### 3. Excited states and the Mott transition

In this section I examine whether there is a Mott transition in the two  $p$ -orbital model, and what its nature is. The method for studying correlated states used here is based on a projection ansatz, where the effects of local spin and density fluctuations are considered. Further details of this method can be found in reference [6]. In brief, the current approach is to calculate the Green's function using the projection method of Mori [9] and Zwanzig [10]. The propagator is projected onto the space spanned by operators  $\{B_1 \dots B_N\}$ , and the Green's function may then be calculated as,

$$\underline{G}(\mathbf{k}, \omega) = \underline{X}[\omega \underline{X} - \underline{F}]^{-1} \underline{X} \quad (7)$$

with

$$F_{\mu\nu} = \langle \Omega | [B_\mu^\dagger, \mathcal{L} B_\nu]_+ \Omega \rangle_c \quad (8)$$

$$X_{\mu\nu} = \langle \Omega | [B_\mu^\dagger, B_\nu]_+ \Omega \rangle_c \quad (9)$$

Note that  $\underline{F}$  and  $\underline{X}$  are Hermitian.  $\mathcal{L}$  is the Liouville operator, defined by  $\mathcal{L}O = [H, O]_-$ . The state  $|\Omega\rangle_c = |1 - \sum_\mu \eta_\mu A_\mu\rangle_c$  is a correlated ground state where the effects of local two-particle excitations have been projected out of the Hartree-Fock state. The subscript  $c$  indicates that these values should be constructed as cumulants (i.e.  $\langle A|B\rangle_c = \langle A^\dagger B \rangle - \langle A^\dagger \rangle \langle B \rangle$ ). This avoids considering unnecessary statistically independent processes. For full details about the cumulant formalism, please refer to Reference [11]. Once matrix 7 has been calculated, the element  $G_{00}(\mathbf{k})$  contains the electron Green's function. The poles of this function define the quasi-particle dispersion.

Following Unger [6], the  $A$  operators are defined as,

$$A_{ij}^1 = 2\delta n_{iI\uparrow}\delta n_{iI\downarrow} \quad (i = j) \quad (10)$$

$$= \delta n_{iI}n_{jI} \quad (i > j) \quad (11)$$

$$A_{ij}^2 = \mathbf{s}_{iI} \cdot \mathbf{s}_{jI} \quad (i > j) \quad (12)$$

in order to take into account local spin (equation 12) and density (equations 10 and 11) fluctuations.  $B$  operators create an additional electron accompanied by a fluctuation (spin or density) and are defined as,

$$B^0 = d_{iI\uparrow}^\dagger \quad (13)$$

$$B_{ij}^1 = 2d_{iI\uparrow}^\dagger \delta n_{iI\downarrow} \quad (i = j) \quad (14)$$

$$= d_{iI\uparrow}^\dagger \delta n_{jI} \quad (i \neq j) \quad (15)$$

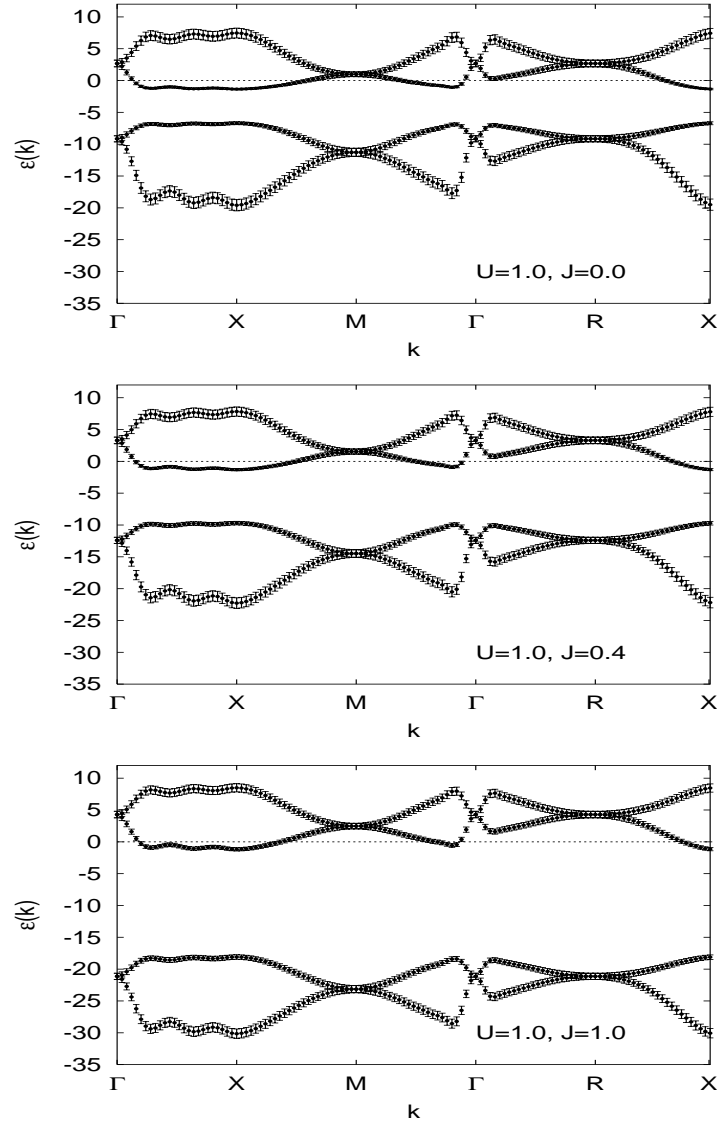
$$B_{ij}^2 = \frac{1}{2}(d_{iI\uparrow}^\dagger S_{jI}^z + d_{iI\downarrow}^\dagger S_{jI}^+) \quad (i \neq j) \quad (16)$$

$$B_{ij}^3 = \frac{1}{2}d_{jI\downarrow}^\dagger d_{jI\uparrow}^\dagger d_{iI\downarrow} \quad (i \neq j) \quad (17)$$

In this way, a total of nine  $B$  operators are defined for the two-band model. Full details of the calculation of the matrix elements required to compute the Green's function in equation 7 are found in reference [6].

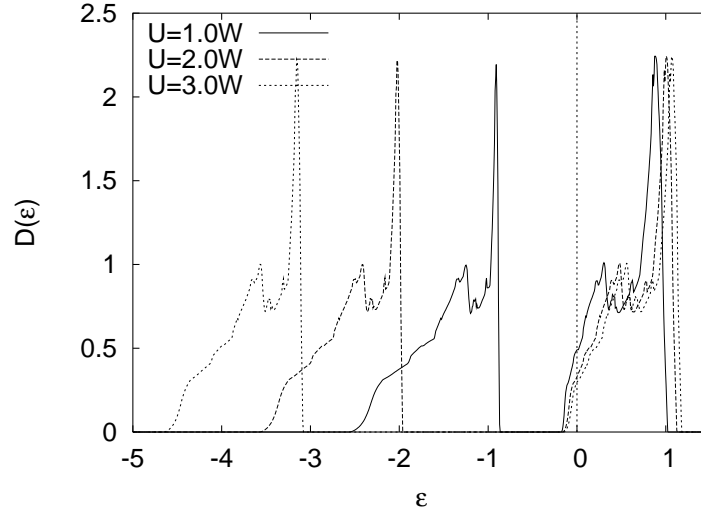
In figure 4, I show the effects of correlations on the band structure of the two band Hubbard model when  $U = W$  for various  $J$ . The correlated dispersion is shown along the main symmetry directions. In can be seen that two almost identical copies of the original dispersion are formed (the top sub-band are approximately the mirror image of the bottom sub-bands in the  $x$ -axis of the graph). The differences between the one and two band models are immediately clear. In the one band case, these bands would split into two identical parts with equal weight, and for sufficiently high  $U$  the bands would untangle and there would be a correlation driven metal insulator (or Mott) transition. In the two-band case, it is no longer necessary that each band splits into lower and upper sub-bands of equal weight. One can see that the weights of the lower sub-band and the second highest sub-band are related in the sense that  $Z_1 + Z_3 = 1$  and similarly  $Z_2 + Z_4 = 1$ , where the subscripts indicate the order of the band from low to high energies. Both geometric effects and more importantly inter-band correlation effects are clearly at work here, since a double-occupied (DO) triplet state can be created in the two band model, allowing the lowest band to absorb the majority of the electrons and for the total energy to be significantly lowered (such a state is prohibited in the one-band model due to the Pauli exclusion principle). The weights  $Z_1 + Z_2 \rightarrow Z_3 + Z_4$  as coupling increases. From bottom to top, the sub-bands are related to: (1) DO electron states with spins in parallel directions, (2) DO electron states with spins in opposite directions, (3) antiparallel DO holes and (4) parallel DO holes. Taking this into account, it is clearly much more difficult to obtain an insulating state in the two-band model, since the weights of the splitting must become symmetric before this takes place.

Figure 5 shows the effect of coupling on the DOS when  $J$  is set to zero. The increase in  $U$  causes a widening of the gap, which is not positioned at the Fermi surface ( $\epsilon = 0$ ). The ratio of  $W_{\text{upper}}$  to  $W_{\text{lower}}$  steadily tends to one. At  $U = 8W$ , the system goes through a dramatic phase transition. Owing to the slightly 1D nature of the  $p$ -orbital chains, a band gap appears for very small  $U < W$ . This is not the Mott-insulating gap (which opens later), but certainly has its origin in correlation



**Figure 4.** Effect of coupling on the bare band structure: (a)  $U=W$ ,  $J=0$ , (b)  $U=W$ ,  $J=0.4W$  and (c)  $U=W$ ,  $J=W$ . The momentum path is taken along the high symmetry directions. “Errorbars” on the plot indicate the residue or quasi-particle weight of the band. The Fermi energy is indicated by the light dotted line. Note that unlike in the simple one band case that corresponds to the Hubbard III approximation [12], bands do not split into sub-bands with equal weight. The only constraint is that  $Z_1 + Z_3 = 1$  and  $Z_2 + Z_4 = 1$ . This is important, since the lower sub-bands are made up of two different weights, and the metal-insulator transition need no longer exist at half-filling. The metal insulator transition will occur when  $Z_1 = Z_4$  and (as implied)  $Z_2 = Z_3$ . The effect of increasing  $U$  and  $J$  is that  $Z_1 \rightarrow Z_4$ . The lower and upper sub-bands narrow, and the Mott gap grows larger. At the transition, the insulating gap is discontinuous.



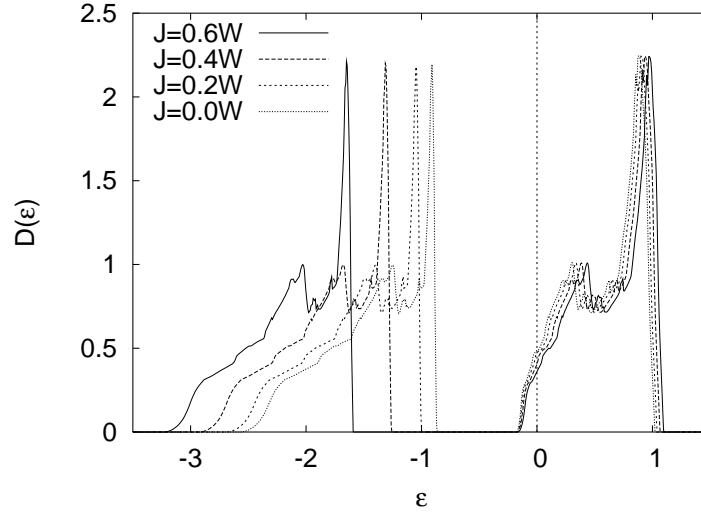


**Figure 5.** Effect of coupling on the DOS.  $J$  is set to zero. The increase in  $U$  effects a widening of the band gap, and of the bands, although the band width,  $W_{\text{upper}}$  calculated from the moments decreases on average. The Mott-transition occurs at  $U = 8W$ . Note that an extremely small  $U$  can open a gap in the density of states. However, the weight of lower and upper bands is not equal, so the low  $U$  gap does not lead to an insulating state. The origin of the low  $U$  gap is almost certainly due to the nature of the model, which to lowest order may be considered to represent interlocking chains, and therefore has some 1D characteristics.

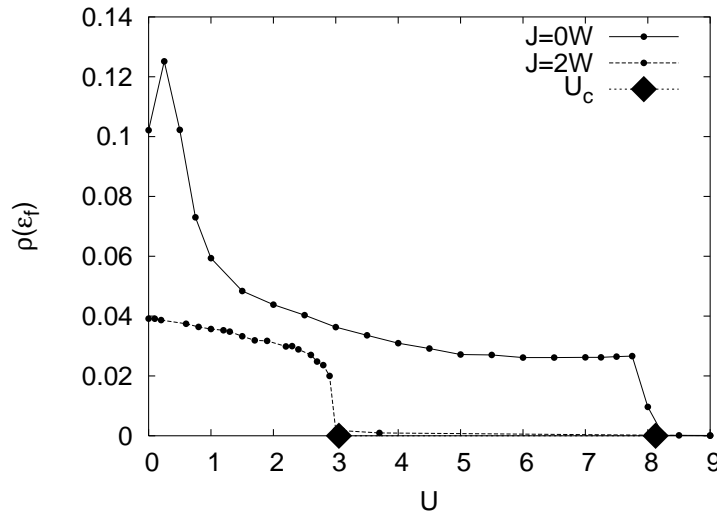
effects. The opening of the Mott gap will be discussed below. Similar effects are seen for positive  $J$ . In figure 6, the effect of spin-spin coupling on the excited states is shown for  $U = W$ . As  $J$  increases, the Mott gap is increased. However, the lower two sub-bands contain less than two electrons, and the Fermi energy lies within the top two sub-bands. As such there are states at the Fermi-surface, and for low  $J$  the system is metallic.

In order to investigate the nature of the Mott transition, I plot the density of states at the Fermi surface,  $\rho(\epsilon_F)$  in figure 7. The upper curve shows the evolution of this property for  $J = 0$ . With slightly increasing  $U$ ,  $\rho(\epsilon_F)$  increases slightly. This is due to the geometry of the bands, and non strictly due to correlation. Above  $U = 0.25W$ , the DOS at the Fermi surface begins to fall, tending to a constant value at around  $U = 6W$ , where presumably the weights of the upper and lower sub-bands have reached a constant value. This persists up to  $U = 8W$ . Then the weights of the upper and lower bands undergo a sudden change so that  $W_{\text{upper}} = W_{\text{lower}}$  and a transition from metal to Mott-Hubbard insulator takes place. For  $J = 2W$ , the transition occurs at a much lower value of  $U = 3W$ , and the weights of the upper and lower sub-bands constantly change up to the transition, since the strong coupling limit has not yet been reached. The critical couplings,  $U_C$  are shown as large diamonds.

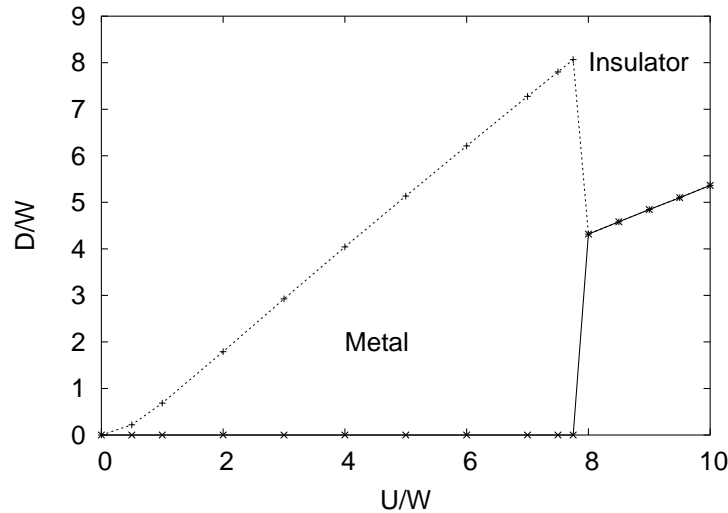
As an additional demonstration of the unusual nature of the Mott-Hubbard transition in this model, I plot the magnitude of the gap in the DOS at  $J = 0$  in figure 8. Starting from very small  $U$ , a gap in the DOS opens approximately linearly in  $U$  up to  $U_c$  (as shown in the faint dotted line). The low  $U$  gap is not positioned at the Fermi-surface, so the system is metallic, although not expected to be a good



**Figure 6.** Effect of exchange on the DOS.  $U = W$  and  $J$  is varied. The energy is in units of the bandwidth. As  $J$  increases, the Mott gap is increased. However, the lower two sub-bands contain less than two electrons, and the Fermi energy lies within the top two sub-bands. As such there are states at the Fermi-surface. A Mott transition is expected at higher (unphysical)  $J$ .



**Figure 7.** Density of states at the Fermi surface  $\rho(\epsilon_f)$  vs  $U$  at half filling with  $J = 0$  and  $J = 2W$ . For the simple model with  $J = 0$ , the onset of the Mott transition is greatly suppressed, with the transition occurring at  $U \sim 8W$ , more that double that expected for the one-band model. Introduction of the spin-spin coupling  $J$  suppresses the DOS at the Fermi surface, pushing the system closer to the Mott state. For  $J = 2W$ , a Mott transition can be seen at  $U = 3W$ . The very small  $\rho(\epsilon_f)$  above  $U = 3W$  is due to small numerical errors.



**Figure 8.** Mott gap when  $J = 0$ . In the metallic state, a gap ( $D$ ) forms just below the Fermi energy. At  $U_c$ , a gap shifts to the Fermi-surface. At the same time, the Mott gap halves. The opening of the Mott gap at the Fermi surface is discontinuous at  $U = 8W$ .

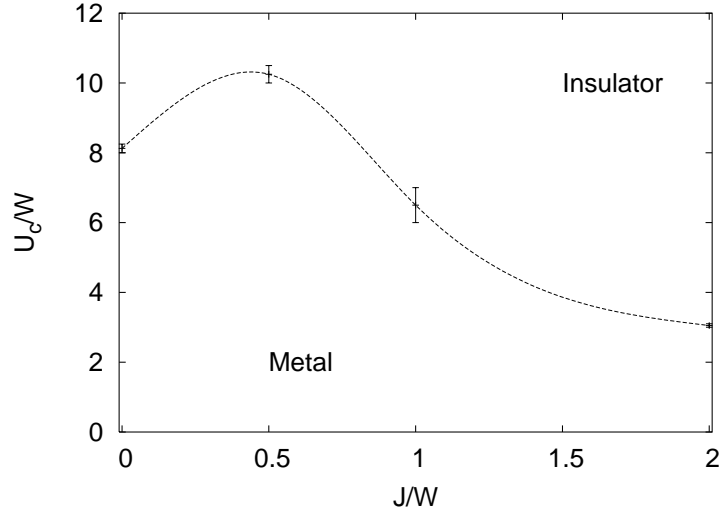
conductor. As previously stated, it is probable that a low  $U$  gap opens since in the non-interacting model, the system of  $p$ -orbitals acts in a similar way to crossed 1D chains. At the critical coupling  $U_c$ , however, the size of the gap suddenly reduces and moves to the Fermi-surface. The system goes through a metal insulator transition. The gap at the Fermi-surface is shown as a thick solid line. The transition is unusual, since the opening of the gap is discontinuous.

In summary, and to close this section, I have investigated the emergence of Mott-Hubbard states in a two-band Hubbard model with degenerate  $p$ -orbitals. The Mott transition is found at a significant  $U_c = 8W$  for the  $J = 0$  model where the inter- and intra- band couplings are equal. This is in agreement with the DMFT results published in references [13, 14] for non-orbital based models where the hopping for different bands may be changed. In reference [13], this increase is attributed to enhanced orbital fluctuations. In this work, such fluctuations can be seen as an asymmetric assignment of weights to certain double occupied and vacant states. As  $J$  is increased, the DOS at the Fermi surface is suppressed. For  $J = 2W$  there is a correlation driven Mott metal-insulator transition at  $U_c = 3W$ . Both of these transitions have the unusual characteristic that the insulating gap opens discontinuously. These results are summarised in figure 9.

#### 4. Orbital anisotropy and band-Mott effects

By changing the relative orbital energies, I also investigate the band-Mott transition. Such a transition is particularly important in the study of correlated electron systems, since one should understand the competition between trivial band insulating effects such as those found in semiconductors, and more complex interaction-driven Mott insulators.

Figure 10 shows the effect of varying orbital energies on the DOS of the 2 band



**Figure 9.** Phase diagram of the two band model at half filling. The lines are a guide to the eye. It can be seen that the critical coupling  $U_c$  is significantly increased in the low  $J$  two-band case. It is expected that this trend will continue as more bands are introduced.

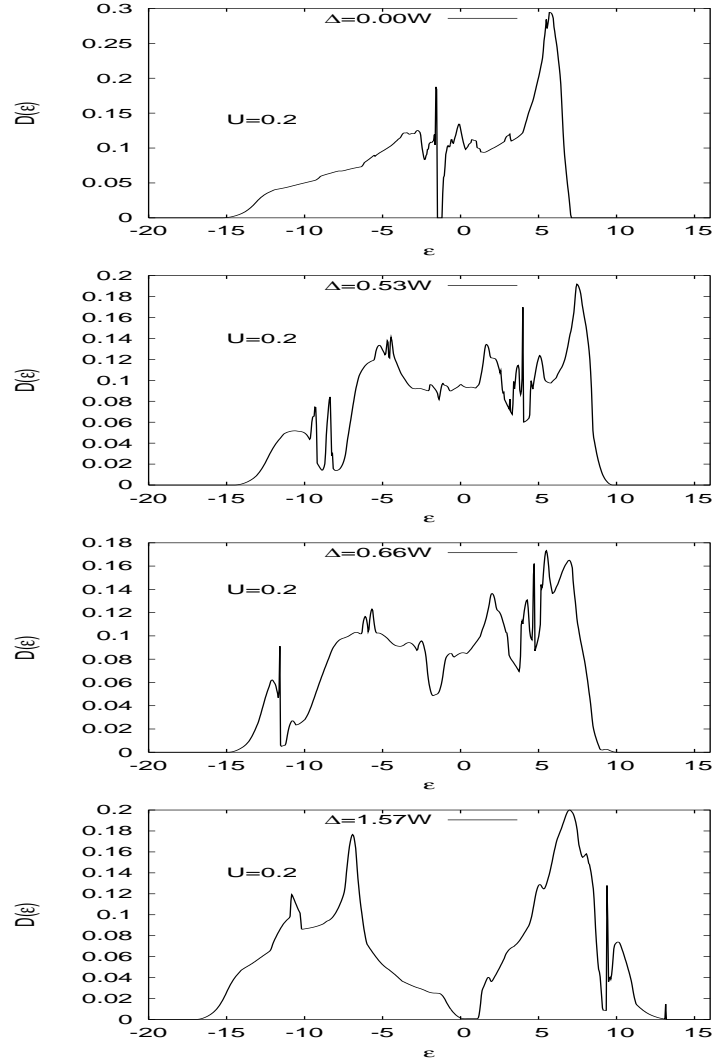
system when  $U = 0.2W$ . The top panel shows degenerate orbital energies, and then moving down, the bands are separated by  $\Delta = 0.53W$ ,  $\Delta = 0.66W$  and  $\Delta = 1.57W$ .

In the top panel a Mott gap (which is not at half-filling) forms. Varying orbital energies acts against this Mott gap. For  $\Delta = 0.53W$ , the conflicting energy scales are similar, and one can see that there is no gapped state. The reason for the disappearance of the gapped state is clear. The lowering of the energy of a single orbital makes the orbital favorable for electrons, so that double occupied states will form. The introduction of a Coulomb repulsion to that orbital means that one of those electrons will be pushed out of that orbital into the higher orbital, and as such electrons can hop again, and a metal results. For  $\Delta = 0.66W$ , orbital ordering starts to dominate, and a gap begins to form close to the Fermi-surface. This gap continues to grow, until the system passes through a metal to band insulator transition at  $\Delta = 1.57W$ .

The metal to band insulator transition is more easily understood, since all the states associated with a band are pushed up in energy until there is a phase transition. Since the states associated with a single band must conserve particle number even in the presence of correlation, then a weight,  $W_1 = 1$  is pushed up, while a weight  $W_2 = 1$  is pushed down. It is therefore clear that for sufficiently large  $\Delta$ , a metal-insulator transition is guaranteed at half-filling. From this mechanism, it is also clear that the gap will always open continuously with respect to  $\Delta$ .

## 5. Conclusions

I have studied the two-dimensional Hubbard model using a projection ansatz that treats the effects of local spin and density fluctuations. A simple model involving two p-orbitals aligned along the  $x$ - and  $y$ -axes was solved, with an on-site Coulomb repulsion  $U$  combined with inter-orbital spin-spin coupling  $J$ . In addition to electron-electron



**Figure 10.** Effect of varying orbital energies on the DOS of the 2 band system. (1) Degenerate orbital energies, (2)  $\Delta = 0.53W$ , (3)  $\Delta = 0.66W$  and (4)  $\Delta = 1.57W$ . Each system is calculated with  $U = 0.2W$ . In the top panel a gap (which is not at half-filling) forms. Varying orbital energies acts against a Mott gap. For  $\Delta = 0.53W$ , one can see that there is no gapped state. For  $\Delta = 0.66W$ , orbital ordering starts to dominate, and a gap begins to form close to the Fermi-surface. This gap continues to grow, until the system passes through a metal- band insulator transition between  $\Delta = 1.5W$ . The opening of the gap is continuous in this case.

interactions, the relative orbital energies were changed by a quantity  $\Delta$  to open a band gap. Since paramagnetic states are considered, correlation-driven insulating states are Mott-Hubbard like [3].

I found that the critical coupling of the Mott transition is much larger in the two-band model than for a simple one-band system. In particular,  $U_c = 8W$  for the two-band case with  $J = 0$ , which is much larger than the simple condition for the one-band model that  $U$  should be greater than the band-width to untangle the bands and open a gap. These results are largely in agreement with the work of Kawakami [13]. The coupling  $J$  acts to suppress  $U_c$ . For all  $J$ , the Mott gap opens discontinuously. I also examined the effects of orbital ordering on the Mott states. The orbital ordering energy  $\Delta$  acts first to close the Mott gap, leading first to an uncorrelated metal, and finally opening a band-insulating gap at  $\Delta \sim 1.43W + U$ .

A non-insulating gap in the DOS is found for low  $U$ . In this regime, the conduction electrons (i.e. those at the Fermi-surface) are found to be associated with only one of the bands. In this sense, the small  $U$  transition could be identified with a primary Mott transition associated with band A which is frustrated by conducting electrons in band B. Such a transition is known as an orbitally selective Mott transition [15]. I note that the sub-band gaps at small  $U$ , are of approximately the same size for both bands, which doesn't completely rule out the possibility that the transition is concurrent [16]. However, reference [16] used a model of non-interacting electrons that neglected hybridisation effects. The inclusion of hybridisation effects makes the model significantly more complicated, and probably leads to the difference in results.

Since a large Coulomb repulsion is required to form an insulating state, even in the case of significant inter-orbital spin-spin coupling, generating Mott-Hubbard states is clearly a difficult task when dealing with real systems beyond the simplified physics of one electron band. The physical origin of this difficulty is that while in the ideal one band model, the band splits into two identical parts with weight  $W_{\text{lower}} = W_{\text{upper}} = \frac{1}{2}$ , this is no longer assured when geometrical effects from real orbitals (including hybridisation), and correlation effects from multiple bands are taken into account. The only constraint is that the total weight of particles in each set of sub-bands (e.g. all sub-bands resulting from band A) is conserved, i.e.  $W_{A,\text{lower}} + W_{A,\text{upper}} = 1$ . It is expected that these effects will become more pronounced as the number of bands increases. Inducing a band insulating state introduces none of these problems, since a whole band (with total  $W_{\text{lower}} + W_{\text{upper}} = 1$ ) is shifted down in energy, until bands no longer overlap, and an insulator is assured.

How do these results relate to real systems? In most materials, especially oxides, several electron bands are important, and orbital energies are shifted due to a combination of geometric effects from the crystal formation and the Hartree–Fock effects of interaction with distant bands (which are well separated in energy). It is therefore important that the effects of correlations in multi-band models competing with orbital energy shifts are well understood. On the basis of the evidence presented in this paper, it is apparent that it is difficult to open a Mott insulating gap in a two-band material, since the critical coupling is so high for realistic values of the spin-spin coupling  $J/U \sim 0.1$ , yet on the other hand, opening band gaps is relatively easy. It is indeed possible that the existence of very strongly correlated band insulators is much more common. Clearly more work should be carried out to assess this situation.

For example, a realistic model of transition metal oxides would take into account the  $e_g$  orbitals which describe the transient electrons in systems such as the CMR manganites. These have the form  $\cos(\theta/2)|x^2 - y^2\rangle \pm i \sin(\theta/2)|3z^2 - r^2\rangle$ . Also,

further lowering of symmetries can change the inter-site hopping along different axes, to generate quasi 1D and 2D systems. Finally, the effect of increasing the number of bands should be considered. Such calculations will form the focus of future work.

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