Insulator-metal transition in the rutile-based VO₂

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The metal-insulator transition (MIT) in paramagnetic VO₂ is studied within LDA+DMFT(IPT), which merges the local density approximation (LDA) with dynamical mean field theory (DMFT). With a fixed value of the Coulomb U = 5.0 eV, we show how the MIT is understood in a new picture: spectral weight transfer accompanying the increase in the displacement of V ion (⊥ c) within the strong correlation scenario. Within this new scenario, we find good quantitative agreement with (i) switch of the orbital occupation of (xy, yz + zx, yz − zx), (ii) thermodynamics, and (iii) the one-electron spectral function in the metallic phase of VO₂. We also compare our results for the total spectral density with other approaches which use QMC to solve the impurity problem of DMFT.

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I. INTRODUCTION

Electron correlation-driven metal-insulator transitions (MIT) in the 3d transition metal (TM) oxides remain a problem of enduring interest in condensed matter physics.¹ Vanadium oxides have proved to be fascinating candidates in this context.² Recent X-ray absorption (XAS) studies³ on V₂O₅ have led to a drastic revision of the traditional picture⁴ of the MIT in this system, forcing a description in terms of a S = 1, multiband model.⁵ Similar behavior is also observed in pressurized Ca₂RuO₄,⁶ suggesting that such a scenario may be a manifestation of the general importance of orbital correlations in TM oxides.

Stoichiometric vanadium dioxide (VO₂) is another example of a system showing a MIT with reduction of temperature. The high-T metallic (M) phase has rutile (R) structure, which changes to monoclinic at the first-order MIT occurring around T_MIT = 340 K. This, along with the observation of spin dimerization along the c-axis,⁸ gave rise to theories linking the MIT to strong electron-lattice coupling (ELC),⁹ where the important role of the antiferroelectric displacement of the V ions (⊥ c) was pointed out. It was suggested that c-axis dimerization of the V-V pairs would open up a gap in the low-T insulating (I) state in the framework of a bonding-antibonding splitting. The M state, accompanied by disappearance of this dimerization, would result from an upward shift of the d_{xy} band (d_{σ} in Ref. 10). In a classic work, a zero-gap insulator was obtained within LDA,¹¹ this study treated structural aspects in full detail. However, the inability to reproduce the observed gap value suggested that inclusion of on-site correlations was necessary. In contrast, in a pioneering work, the importance of electronic correlations, along with that of the antiferroelectric displacement of V ions from their c-axis positions in driving the MIT was emphasized.¹² From a detailed perusal of experimental results known at that time, it was argued that c-axis spin dimerization is a consequence of the MIT driven by electronic correlations in concert with the antiferroelectric displacements. Subsequently, a model calculation explicitly realized this suggestion, but with unrealistically small model parameters. On the experimental side, the observation of anomalous (correlation driven) features¹³–¹⁵ and results from magnetic measurements¹⁶ finding local moments in V₁₋ₓCr₂O₅, required a correlation based scenario. Simultaneously, observation of only a modest mass enhancement in the R phase seemed to suggest that while correlations were undoubtedly present, they did not play a crucial role in the MIT. In the light of this conflict, the origin of the PI state as well as the mechanism of the MIT is an open and controversial issue.

Recent (unpublished) XAS results¹⁷ show that the abrupt MIT in VO₂ is accompanied by a hysterensis in occupation of different t₂g orbitals, directly confirming the importance of orbital correlations in a multi-band situation.⁵ Recent photoemission measurements show a large spectral weight transfer from high- to low-energies, on a scale of O(2 eV), across the MIT. Further, this character of the MIT, which is driven by a sudden increase in carrier density rather than their mobility, is shown very clearly by time-delay measurements.¹⁸ More recently, Lim et al.¹⁹ found the MIT to be strongly first order by I-V measurements on thin films. Very interestingly, micro-Raman scattering experiment clearly shows that this electric field driven Mott transition is not accompanied by any structural transition, in contrast to the usual T driven one, strongly suggesting the Mott-Hubbard scenario. These observations put particularly strong constraints on an acceptable theory of the MIT for VO₂: (i) it should be able to describe this switch in orbital occupation at the MIT, (ii) the metallic phase should be moderately correlated (see, however,¹⁵), and, (iii) the insulator should be of the Mott-Hubbard type, accompanied by c-axis dimerization of V⁴⁺,V⁴⁺ pairs, and the MIT itself should be first-order, consistent with Ref. 18.

In this article, we discuss a concrete theoretical scenario, extending¹⁰,¹² earlier works in the light of the above requirements. Using the recently developed ab initio LDA+DMFT scheme, we show how a consistent treatment of strong, dynamical multi-orbital correlations
along with the antiferroelectric displacements of V in the real LDA bandstructure leads to a unified understanding of the MIT in VO$_2$. We also compare our results with other, recent LDA+DMFT work which uses quantum Monte Carlo (QMC) method to solve the impurity problem of DMFT. Finally, we show how very good quantitative agreement with PES, XAS, thermodynamic and magnetic measurements is obtained. Our results support the Mott-Hubbard picture of the MIT in VO$_2$, where the Peierls instability arises subsequent to the M-I transition.

II. MODEL AND SOLUTION

We start with the LDA bandstructure of VO$_2$ in the monoclinic crystal structure corresponding to the insulating phase. The LDA DOS, computed using the known value of the antiferro-electric displacement of V$^{4+}$ ions ($\epsilon$, giving the splitting $\Delta_{\alpha\beta}$ between the $xy, yz \pm zx$ orbitals at the local level) (Fig. 1) shows interesting features: the lowest lying $xy$ (in the $M$ notation) band is the most heavily populated, while the $yz \pm zx$ bands are less populated. The bonding-antibonding splitting is clearly visible in the results, which also show that the total bandwidth is about $W \approx 2.3$ eV, contrary to much smaller previous estimates based on model calculations. Except for their inability to reproduce the Mott gap, these LDA results agree with Goodenough’s arguments. As emphasized by Mott, it is inconceivable that $\epsilon$ alone could open up a charge gap ($E_G \approx 0.6$ eV), this requiring proper incorporation of correlation effects.

Thus, the LDA (bandstructure) part of the Hamiltonian is

$$H_0 = \sum_{k\alpha\beta\sigma} \epsilon_{\alpha\beta}(k)c_{k\alpha\sigma}^\dagger c_{k\beta\sigma} + \sum_{i\alpha\sigma} \epsilon_{i\alpha\sigma} n_{i\alpha\sigma}$$  

(1)

where $\alpha, \beta = xy, yz + zx, yz - zx$. To avoid double counting of interactions already treated on the average by LDA, we follow to write

$$H_{LDA}^{(0)} = \sum_{k\alpha\beta\sigma} \epsilon_{\alpha\beta}(k)c_{k\alpha\sigma}^\dagger c_{k\beta\sigma} + \sum_{i\alpha\sigma} \epsilon_{i\alpha\sigma} n_{i\alpha\sigma},$$  

(2)

where $\epsilon_{i\alpha\sigma} = \epsilon_{i\alpha\sigma} - U(n_{i\alpha\sigma} - \frac{1}{2}) + \frac{1}{2}J_H(n_{i\alpha\sigma} - 1)$, with $U, J_H$ as defined below, and the full Hamiltonian is

$$H = H_{LDA}^{(0)} + U \sum_{i\alpha} n_{i\alpha\uparrow} n_{i\alpha\downarrow} + \sum_{i\alpha\beta\sigma} U_{\alpha\beta} n_{i\alpha\sigma} n_{i\beta\sigma}$$  

(3)

$$- J_H \sum_{i\alpha\beta} S_{i\alpha} \cdot S_{i\beta}.$$  

Constrained LDA calculations give $U \approx 4.5$ eV, $J_H = 1.0$ eV and $U' = U_{\alpha\beta} = (U - 2J_H) = 2.5$ eV. Given the uncertainty in the precise estimation of $U$, we choose $U = 5.0$ eV in the calculations. Considering only the $t_{2g}$ manifold, the PM/para-orbital phase, and working in the basis which diagonalises the LDA density matrix, we have $G_{\alpha\beta\sigma\sigma}(\omega) = \delta_{\alpha\beta}\delta_{\sigma\sigma}G_\sigma(\omega)$ and $\Sigma_{\alpha\beta\sigma\sigma}(\omega) = \delta_{\alpha\beta}\delta_{\sigma\sigma}\Sigma_\sigma(\omega)$.

In the $t_{2g}$ sub-basis, a DMFT solution involves (i) replacing the lattice model by a multi-orbital, asymmetric Anderson impurity model, and (ii) a selfconsistency condition requiring the impurity propagator to be equal to the local ($k$-averaged) Green function of the lattice, given by

$$G_{\alpha}(\omega) = \frac{1}{V_B} \int d^3k \left[ \frac{1}{(\omega + \mu)1 - H_{LDA}^{(0)}(k) - \Sigma(\omega)} \right]_\alpha.$$  

(4)

Using the locality of $\Sigma_{\alpha\beta}$ in $d = \infty$, we get $G_{\alpha}(\omega) = G_{\alpha}^0(\omega - \Sigma_{\alpha}(\omega))$. Further, since $U_{\alpha\beta}, J_H$ scatter electrons between the $xy, yz + zx, yz - zx$ bands, only the total number, $n_{t_{2g}} = \sum_{\alpha} n_{t_{2g},\alpha}$ is conserved in a way consistent with Luttinger’s theorem.

To solve the impurity problem of DMFT, we use the iterated perturbation theory (IPT), generalized to the case of $t_{2g}$ orbitals for arbitrary filling. The local propagators are given by

$$G_{\alpha}(\omega) = \frac{1}{N} \sum_{k} \frac{1}{\omega - \Sigma_{\alpha}(\omega) - \epsilon_{k\alpha}}.$$  

(5)

Local dynamical self-energies $\Sigma_{\alpha}(\omega)$ are computed within the extended multi-orbital iterated-perturbation theory (MO-IPT) which generalizes the IPT for the one orbital case to the multi-orbital situation, for any temperature and band-filling. Explicitly,

$$\Sigma_{\alpha}(\omega) = \frac{\sum_{\gamma} A_{\alpha\gamma} \Sigma_{\gamma}^{(2)}(\omega)}{1 - \sum_{\gamma} B_{\alpha\gamma} \Sigma_{\gamma}^{(2)}(\omega)}.$$  

(6)

where, for example,
\( \Sigma_{\alpha\gamma}(i\omega) = \frac{U^2_{\alpha\gamma}}{\beta^2} \sum_{n,m} G^0_{\alpha}(i\omega_n)G^0_{\gamma}(i\omega_m)G_{\alpha}(i\omega_n + i\omega_m - i\omega) \)

and \( G^0_{\alpha}(\omega) = \frac{1}{\omega + \mu_{\alpha} - \Delta_{\alpha}(\omega)} \). The multi-orbital dynamical bath \( \Delta_{\alpha}(\omega) \) function is determined using the DMFT self-consistent condition which requires that the local impurity Green function to be equal to the local Green function of the lattice (Eq. (5)). Finally, in Eq. (6),

\[
A_{\alpha\gamma} = \frac{n_{\alpha}(1 - 2n_{\alpha}) + D_{\alpha\gamma}[n]}{n_{\alpha}^0(1 - n_{\alpha}^0)}
\]

and,

\[
B_{\alpha\gamma} = \frac{(1 - 2n_{\alpha})U_{\alpha\gamma} + \mu_{\alpha} - \mu_{\alpha}^0}{2U^2_{\alpha\gamma}n_{\alpha}^0(1 - n_{\alpha}^0)}
\]

Here, \( n_{\alpha} \) and \( n_{\alpha}^0 \) are particle numbers determined from \( G_{\alpha} \) and \( G_{\alpha}^0 \) respectively, and \( D_{\alpha\gamma}[n] = \langle n_{\alpha}n_{\gamma} \rangle \) is calculated using

\[
\langle n_{\alpha}n_{\gamma} \rangle = \langle n_{\alpha} \rangle \langle n_{\gamma} \rangle - \frac{1}{U_{\alpha\gamma}} \int f(\omega) Im[\Sigma_{\alpha\gamma}(\omega)G_{\alpha}(\omega)]d\omega.
\]

The last identity in Eq. (9) follows directly from the equations of motion for \( G_{\alpha}(\omega) \). These equations satisfy the Luttinger sum rule, and reproduce the first few moments of the spectral functions, the renormalized value of the distortion \( \Delta_{\alpha\beta} \) leads to large changes in spectral weight via DMFT in the multi-orbital situation, and, at a critical \( n_{||} \), to an abrupt (first-order) transition to a metallic phase (Fig. 2, dashed lines, computed for \( T = 0.03 \) eV). Interestingly, the \( d_{||} \) DOS still represents insulating behavior, while the \( d_{\pi} \) DOS exhibits characteristic metallic behavior, providing an explicit realization of the two-fluid scenario proposed earlier to describe the general problem of MIT. In accord with the above argument, the renormalized \( \Delta_{\alpha\beta}^M \simeq -0.29 \) eV, corresponding to a reduction in \( \Delta_{\alpha\beta} \), in full agreement with Mott.\(^{10}\) The difference \( \delta = \Delta_{\alpha\beta}^I - \Delta_{\alpha\beta}^M = 0.46 \), in good agreement with the value of \( 0.5 - 0.6 \) from cluster calculations.\(^{10}\) Moreover, this agrees with the orbital splitting assignment in the M phase,\(^{9,10,20}\) where the \( d_{\pi} \) band(s) lies lower than the \( d_{||} \) band. Finally, the orbital occupations in the M phase are found to be \( (n_{||}, n_{\pi}) = (0.34, 0.33, 0.33) \) respectively, in very good semiquantitative agreement with recent XAS results.

Based on these results, the abrupt MIT in VO\(_2\) is un-

![FIG. 2](image-url)
derstood as follows. A decrease in the LDA value of $n_\parallel$ leads to an effective reduction in $\Delta^I$ (caused by Hartree shifts due to $U_{\alpha\beta}$) leading to an effective increase in $n_\pi$, and, more importantly, to large changes in dynamical SWT from high- to low energy, driving the first order MIT. The converged values of $n_\pi$ (obviously different from the trial values) vary in a way qualitatively consistent with indications from recent XAS measurements. Thus, in our picture, the MIT is driven by (i) abrupt changes in $n_\parallel$, $n_\pi$ and $\Delta_{\alpha\beta}$ due to large change in dynamical SWT, and, (ii) an increase in the carrier concentration, rather than their mobility, consistent with time-delay measurements.\(^{18}\)

[GRAPHIC]

FIG. 3. (color online) The integrated photoemission lineshapes for the PI (solid) and PM (dashed) phases within LDA+DMFT for $U = 5.0$ eV. The LDA result is the dot-dashed line.

Given the relatively wide $t_{2g}$ bands in the LDA (contrast with Ref. 12, where the bandwidths, as well as $U, U_{\alpha\beta}, J_H$ were severely underestimated), correlation induced mass enhancement is found to be moderate. Indeed, from the self-energy (not shown), the average effective mass enhancement factor is $m*/m_0 \approx 3.0$, in full accord with that extracted from reflectance studies.\(^{27}\) Clearly, this enhanced mass comes solely from the $d_\pi$ band (this is the only band showing “metallic” behavior).\(^{10}\) Further, the high-$T$ static spin susceptibility is enhanced by the same factor of 3 coming from renormalization effects of multi-orbital correlations, in contrast to the Stoner mechanism discussed before in Ref. 10. These results can be interpreted to mean a moderate renormalization caused by the additional screening provided by the wide $d_\pi$ bands in the M phase.

In Fig. 3, we show the integrated photoemission (PES) spectra calculated in both the I and the M phases. Comparing our results with published experimental work,\(^{14}\) very good semi-quantitative agreement between theory and experiment is seen. In this context, we emphasize that a certain amount of caution should be exercised while comparing theory to experiment because (i) reduced co-ordination at the surface would normally enhance correlation effects, decreasing the DOS at $E_F$, and (ii) the surface of VO$_2$ is known to show insulating features (Ref. 14). Incorporating spin-Peierls effects in the PI phase will also change the PES lineshape in the PI phase somewhat; this is left for the future. With these caveats in mind, the overall agreement is strikingly good, and, in particular, the transfer of spectral weight across the MIT is faithfully reproduced by theory.

In particular, in our picture, the small peak in the metallic phase is not a quasicoherent Fermi liquid (FL) peak, but part of the tail of the $d_{yz\pm xx}$ bands (from Fig. 2) pulled down below $E_F$ in the PM phase, as described above. More detailed orbital-selective spectroscopic investigations are needed to confirm this picture.\(^{28}\) This is also consistent with the absence of a $T^2$ term in the $dc$ resistivity, which is known\(^{15}\) to follow a linear-in-$T$ behavior for $330 \text{ K} < T < 840 \text{ K}$. We notice that a FL peak in PES would contradict the incoherent, linear-in-$T$ (non-FL) resistivity. In any case, in correlated systems on the verge of a Mott transition, such a FL resonance should be visible, if at all, only at very low temperatures, and is rapidly washed off with increasing $T$.

IV. COMPARISON WITH LDA+DMFT(QMC) RESULTS

We turn now to a comparison of our work with other, recent approaches which use QMC to solve the impurity problem of DMFT.\(^{29-31}\) First, we clearly see in Fig. 4 that the QMC calculations resolve a huge peak near $E_F$. Though a miniscule pseudogap can be discerned in Ref. 29, a direct comparison between both LDA+DMFT(QMC) results with the corresponding LDA ones clearly shows that the many-body renormalised DOS, $\rho(E_F)$ at the Fermi surface, coincides with the corresponding LDA DOS, even at $T = 770 \text{ K}$. (Note that the QMC calculations done at $T \approx 500 \text{ K}$ are also pinned to the same value at $E_F$). This is clearly problematic: let us recall that the Friedel Luttinger sum rule implies $\rho(E_F) = \rho_{LDA}(E_F)$ only at $T = 0$ in $d = \infty$. Further, in a DMFT framework, this pinned (at $T = 0$) feature actually ceases to exist above the lattice coherence scale, $T_{coh}$, which is quite small near a correlation-driven MI transition. In the LDA+DMFT framework, such a pinned feature can only be associated with a correlated FL peak. Its persistence up to $T = 770 \text{ K}$ (QMC) is thus in direct conflict with the bad-metallic, linear-in-$T$ resistivity observed from much lower $T (= 340 \text{ K})$ in VO$_2$. Optical measurements further confirm this,\(^{26}\) no coherent Drude peak is observed in the PM phase.

The pinning observed in LDA+DMFT(QMC) work is thus very hard to justify, both on theoretical and experimental grounds. Further, explicit consideration of
inter-site V-V interactions (dimerisation) within cluster DMFT would normally cause a low-energy pseudogap to appear around $E_F$, making any pinning impossible, even at $T = 0$. Clearly, our results do not suffer from this conflict, and are moreover in excellent quantitative accord with PES/XAS results, as well as with the effective mass enhancement estimated from optics/thermodynamics, as discussed before. To compare various approaches, we show in Fig. 4 our result, together with those obtained from LDA+DMFT(QMC)\textsuperscript{29–31} in comparison with recent experimental results. While our result quantitatively describes the full spectral function from $-3.0 \leq \omega \leq 1.2$ eV, the LDA+DMFT(QMC) result does not capture the detailed lineshape correctly over the whole range.

![Fig. 4. Comparison of theoretical LDA+DMFT(IPT) and LDA+DMFT(QMC) result for the total one-electron spectral function in the metallic phase of VO$_2$ to the experimental results taken from Ref. 33 (for PES) and from Ref. 34 (for XAS). The LDA+DMFT(QMC) results are taken from: Ref. 29 (\textit{a}) $[T = 770 \text{ K}]$, Ref. 31 (\textit{b}) $[T = 770 \text{ K}]$, and Ref. 30 (\textit{c}) $[T \approx 500 \text{ K}]$.](image)

What are the sources of the discrepancy between our results and the LDA+DMFT(QMC) ones? There are two important differences between our approach compared to the LDA+DMFT(QMC) works: The LDA+DMFT(QMC) papers derive the many-body density of states (DOS) in the two phases (dimerised/metallic) by using the corresponding LDA DOS separately for each phases, and using DMFT(QMC) to study dynamical correlation effects in each phase. Thus, the two phases can be studied separately, but it is difficult to see how the first-order transition between the two could be derived this way.

We argue that this is problematic because the MI transition in the actual correlated system is driven by large changes in transfer of dynamical spectral weight in response to small changes in the renormalised LDA parameters. In a multi-orbital system, these (the AFE distortion in VO$_2$) are themselves modified in a priori unknown (sometimes non-trivial) ways by electronic correlations. Our approach is to search for an instability from the Mott insulating (MI) phase (corresponding to one solution of the DMFT equations) to the paramagnetic metallic phase (the second solution of the DMFT equations) as a function of the renormalised AFE distortion, as explained above.

Finally, another source of discrepancy is the use of different LDA DOS: we have used the $t_{2g}$ DOS as derived by Korotin \textit{et al.}\textsuperscript{20} while the LDA+DMFT(QMC) works use downfolded LDA DOS. As is clear from a direct comparison between the two LDA results (see Fig. 5), downfolding the LDA DOS results in an appreciably larger bonding-antibonding feature in the $d_{xy}$ DOS. Clearly, the details of the many-body DOS depend sensitively on using/not using this device, and the difference between our result and those in other works is partly attributable to this difference in the corresponding LDA DOS.

![Fig. 5. LDA partial density of states for the $d_{xy}$ (top) and $d_{yz} \pm i d_{zx}$ (bottom) orbitals, obtained from Ref. 20 (black) and from Ref. 29 (blue). The latter obtained after downfolding.](image)
existence of long- and short V-V distances along c with concomitant c-axis spin dimerization would follow as a consequence of the I phase and would not be responsible for driving the MIT (incorporation of $\Delta_{ab}$ into LDA does not yield the I phase). An analysis along the lines of Ref. 12 is possible, but requires more work within our formulation. The resulting c-axis spin dimerization in the I phase should in principle explain the magnetic properties in the I phase. This would also have the generic effect of increasing the gap ($E_G$) to values closer to the experimental value of 0.6 eV. More work is needed to make quantitative comparison, and this is left for the future.

V. CONCLUSION

In conclusion, in the light of the theoretical constraints imposed by various experimental results, we have studied the T-driven MIT accompanied by abrupt changes in orbital occupations using the ab-initio LDA+DMFT scheme. In complete accord with Mott’s ideas, the MIT is shown to be of the Mott-Hubbard type, driven by an increase in the itinerant carrier density. The orbital occupations in the PM phase are found to be in excellent semiquantitative agreement with indications from recent polarized XAS studies. Furthermore, good quantitative agreement with thermodynamic data and the one-electron spectrum in both the I and M phases is obtained in the same picture, providing a unified description of the physics of VO$_2$ across the MIT. Such a description can have a wider application to other systems where strong multi-orbital correlations in concert with structural details drive a first-order MIT under external perturbations.

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