# Two aspects of the Mott-Hubbard transition in Cr-doped V2O3

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# Two aspects of the Mott–Hubbard transition in Cr-doped $V_2O_3$

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**Abstract**

The combination of bandstructure theory in the local density approximation with dynamical mean-field theory was recently successfully applied to $V_2O_3$—a material which undergoes the famous Mott–Hubbard metal–insulator transition upon Cr doping. The aim of this short paper is to emphasize two aspects of our recent results: (i) the filling of the Mott–Hubbard gap with increasing temperature, and (ii) the peculiarities of the Mott–Hubbard transition in this system which is not characterized by a divergence of the effective mass for the $a_{1g}$-orbital.

A paradigm of electronic correlations is the Mott–Hubbard metal–insulator transition, triggered by an increasing ratio of Coulomb interaction over bandwidth ($U/W$). Experimentally, it is realized in paramagnetic $V_2O_3$ upon Cr-doping or decreasing pressure. Theoretically, the combination of the local density approximation and dynamical mean-field theory (LDA + DMFT [1]) was successfully employed to this system recently [2], stimulating new experiments [3]. Here we restrict ourselves to two fascinating aspects of the transition: (i) the filling of the Mott–Hubbard gap with increasing temperature [3] and (ii) the peculiarities of the Mott–Hubbard transition due to the inequivalence of the $a_{1g}$- and $e_g$-orbitals [2].

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(i) *Filling of the Mott–Hubbard gap with increasing temperature*: A feature genuine to a Mott–Hubbard insulator is that the zero temperature ($T$) Mott–Hubbard gap is filled with spectral weight when $T$ is increased. In contrast, for a semiconducting or band insulator a gap stays a gap with increasing $T$; only some electrons are statistically transferred across the gap because of finite $T$. How can we understand this non-intuitive feature of the Mott–Hubbard insulator? Let us follow the two paths for metallic $V_2O_3$ and insulating $(V_{0.972}Cr_{0.028})_2O_3$ in the phase diagram Fig. 1a. If we consider a paramagnet instead of the antiferromagnetic insulator (AFI) at zero temperature, the paramagnetic metal (PM) is a Fermi liquid with a central quasiparticle resonance (point $0'$) and the insulator (PI) is gapped (point 0). This picture changes only slightly if we increase $T$ to points $1'$ and 1. When $T$ is however further increased (to point $2'$) one enters the crossover regime, the quasiparticle peak fades away, and the lifetime becomes too short to speak of a quasiparticle peak anymore. Since the insulator and the metal are not distinct phases in the crossover regime, we see the Mott–Hubbard gap being filled with incoherent (short life-time) spectral weight as one goes from point 1 to 2. This weight may be interpreted as a smeared out quasiparticle peak.

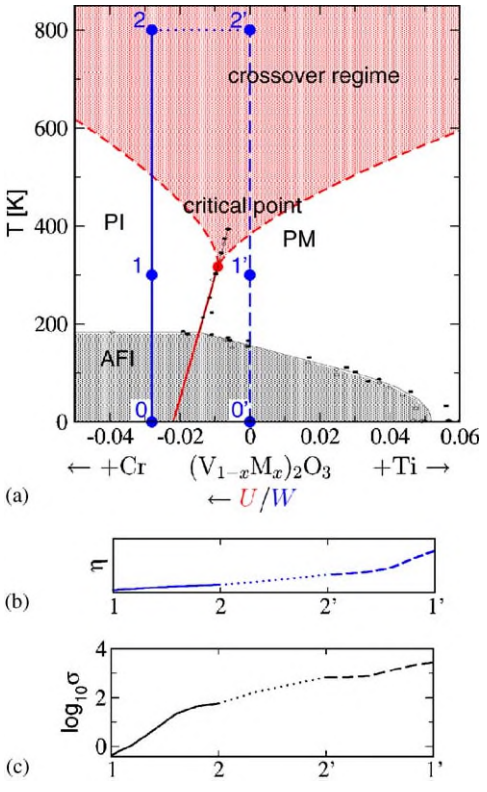


Fig. 1. (a) Experimental (black/white) and DMFT (colors) phase diagram of $V_2O_3$; (b) order parameter of the DMFT Landau theory and (c) logarithm of the experimental conductivity (in units of $(\Omega\,\mathrm{cm})^{-1}$) along the paths of (a) (reproduced from Ref. [3] with (c) read off from Ref. [4]).

In Fig. 1b, the calculated [3] order parameter $\eta$ of the DMFT Landau theory [5] is plotted. Since $\eta$ corresponds to the spectral weight at the Fermi energy, it shows in detail the reduction of the metallic quasiparticle peak and the filling of the Mott–Hubbard gap along the lines from point $1'$ to $2'$ and from 1 to 2, respectively. As was pointed out in Ref. [3], this behavior is indeed seen in the experimental conductivity (Fig. 1c). Mo et al. [3] particularly observed for the first time the filling of the Mott–Hubbard gap with increasing $T$ by photoemission spectroscopy, see Fig. 2, ascertaining the DMFT prediction.

(ii) *Peculiarities of the Mott–Hubbard transition*: Let us now turn to a different aspect of the Mott–Hubbard transition which stems from the

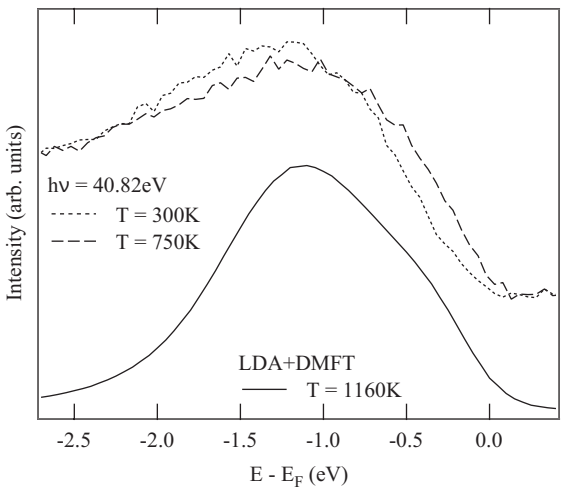


Fig. 2. Photoemission spectra showing the transfer of spectral weight into the Mott–Hubbard gap with increasing $T$ and LDA + DMFT prediction [2] (reproduced from [3]).

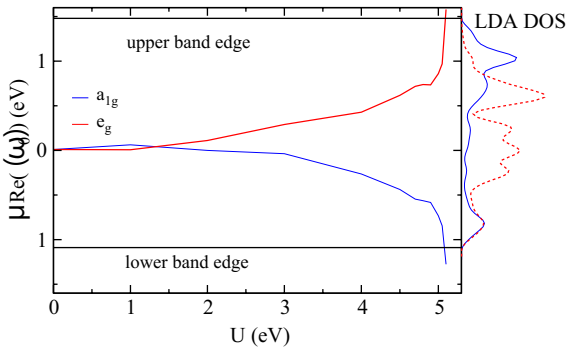


Fig. 3. The LDA + DMFT effective chemical potential $\mu - \Re\Sigma_m(\omega_0)$, for the $a_{1g}$- and $e_g^\pi$-orbitals (taken at the lowest Matsubara frequency $\omega_0$) moves out of the band edges of the LDA DOS at the critical $U$ for the Mott–Hubbard transition (reproduced from Ref. [2]).

orbital degrees of freedom. Within the Fermi-liquid metallic phase of $V_2O_3$, the Green function is given by

$$G_m(\omega) = \int \mathrm{d}\varepsilon \, \frac{ZN_m^0(\varepsilon)}{\omega + Z(\mu - \Re\Sigma_m(0) - \varepsilon)} \qquad (1)$$

at low frequencies $\omega$. Here, $N_m^0(\varepsilon)$ is the non-interacting (LDA) density of states (DOS) for $m = e_g^\pi$ or $m = a_{1g}$, $\Sigma_m$ denotes the self-energy and $Z_m = (1 - \partial\Re\Sigma_m(\omega)/\partial\omega\,|_{\omega=0})^{-1}$ the quasiparticle weight. In the one-band Hubbard model, the Mott–Hubbard transition is characterized by $Z \to 0$ at the critical value of $U$, or equivalently a divergence of the effective mass. The width of the quasiparticle peak goes to zero. Keller et al. [2] showed in their LDA + DMFT calculation that the Mott–Hubbard transition in $V_2O_3$ is actually different. While $Z_{e_g^\pi} \to 0$ for the two $e_g^\pi$-bands, $Z_{a_{1g}} \nrightarrow 0$ for the $a_{1g}$-band at the Mott–Hubbard transition. How can the $a_{1g}$-band then become insulating? Looking at Eq. (1), we see that there is another possibility consistent with the Fermi-liquid metallic phase. The height of the quasiparticle peak is given by $N_m(\mu - \Re\Sigma_m(0))$. As is shown in Fig. 3, $\mu - \Re\Sigma_m(0)$ moves out of the non-interacting DOS at the Mott–Hubbard transition. Hence, the height of the quasiparticle peak goes to zero. For the $a_{1g}$ quasiparticle peak, the height goes to zero at fixed width (which is already strongly reduced compared to $U = 0$). For the $e_g^\pi$-orbitals, the transition is characterized by a combined shrinking of width and height.

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