Combined GW and dynamical mean-field theory: Dynamical screening effects in transition metal oxides

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Abstract – We present the first dynamical implementation of the combined GW and dynamical mean-field scheme (“GW + DMFT”) for first-principles calculations of the electronic properties of correlated materials. The application to the ternary transition metal oxide SrVO₃ demonstrates that this scheme inherits the virtues of its two parent theories: a good description of the local low-energy correlation physics encoded in a renormalized quasi-particle band structure, spectral weight transfer to Hubbard bands, and the physics of screening driven by long-range Coulomb interactions. Our data is in good agreement with available photoemission and inverse photoemission spectra; our analysis leads to a reinterpretation of the commonly accepted “three-peak structure” as originating from orbital effects rather than from the electron addition peak within the t₂g manifold.

Describing electronic excitations of materials with strong electronic Coulomb interactions remains one of the challenges of modern condensed-matter theory [1]. Photoemission satellite features, quasi-particle mass renormalizations or — in the strong-coupling limit — the localization of electrons are phenomena well beyond band theory. Within effective low-energy models, such as the Hubbard or Anderson lattice model, insight has been gained into the low-energy physics of correlated materials on a qualitative level. However, when relating this knowledge to specific materials, attempted a quantitative description, several challenges persist: The first one is a question of energy scales: in fact, much of the physics of interest in correlated materials takes place on the scale of several eV, well beyond what is captured within a low-energy description. Optical properties of transition metal oxides, to cite a specific example, are determined by the onset of optical transitions involving ligand states already at scales of only a few eV. A second issue is the determination of the model parameters, e.g., the effective low-energy hopping parameters and Coulomb interactions, in particular the local “Hubbard U”. These two issues are in fact intimately related, since high-energy screening processes renormalize these parameters, and an appropriately downfolded low-energy model should take this into account [2–7].

In this letter, we present the first dynamical implementation of a combined GW and dynamical mean-field (“GW + DMFT”) scheme that addresses the above issues, by treating explicitly both dynamical Coulomb interactions on the “correlated” manifold of orbitals and corrections to the band structure of degrees of freedom that live on higher-energy scales. The application to a well-studied correlated metal, SrVO₃, shows some expected features: a renormalization of the quasiparticle band structure, the formation of a lower Hubbard band and the correction of the position of the oxygen p-states. It also leads to less expected features, namely the absence of a clearly
distinguishable upper Hubbard band in the total spectral function along with a reinterpretation of the feature seen at about 2.7 eV in inverse photoemission that we associate with the $e_g$ states. This attribution is in agreement with cluster model calculations [8] and allows to resolve apparent contradictions between cluster and dynamical mean-field methods for this compound. In the orbital-resolved spectral function we furthermore predict additional satellite features induced by the frequency dependence of the effective Coulomb interaction.

The combined GW + DMFT scheme was proposed a few years ago, in order to avoid the ad hoc nature of the Hubbard parameter and the double counting inherent to conventional combinations of dynamical mean-field theory with density functional theory in the local density approximation (so-called “LDA+DMFT” schemes [9,10]). The starting point is Hedin’s GW approximation (GWA) [11], in which the self-energy of a quantum many-body system is obtained as a product of the Green’s function $G$ and the screened Coulomb interaction $W = e^{-1}V$. The dielectric function $\epsilon$, which screens the bare Coulomb potential $V$, is in–within a pure GW scheme—obtained from the random phase approximation. The GW + DMFT scheme, as proposed in [12], combines the first-principles description of screening inherent in GW methods with the non-perturbative nature of DMFT, where local quantities such as the local Green’s function are calculated to all orders in the interaction from an effective reference system (“impurity model”). In DMFT, one imposes a self-consistency condition for the one-particle Green’s function, namely, that its on-site projection equals the impurity Green’s function. In GW + DMFT, the self-consistency requirement is generalized to encompass two-particle quantities as well, namely, the local projection of the screened interaction is required to equal the impurity screened interaction. This in principle promotes the Hubbard $U$ from an adjustable parameter in DMFT techniques to a self-consistent auxiliary function that incorporates long-range screening effects in an $ab initio$ fashion. Moreover, the theory provides momentum dependence to quantities (such as the self-energy) that are local within pure DMFT. Despite these conceptually attractive features, however, no dynamical implementation, even at the non–self-consistent level has been achieved so far (see, however, the static dynamical implementation, even at thenon–self-consistent level) [8,24–36]. Recent works include, e.g., studies of surface effects [37], kink structures in the momentum-resolved spectral function [38–40], or non-local correlation effects [41,42] in relation to laser ARPES [43] which finds a “dip” at the Fermi level or a maximum of the quasi-particle peak slightly below (at around $-0.2$ eV). The experimentally observed quasi-particle weight is about 0.5–0.6 [24,44–50], with the remaining spectral weight being carried by a photoemission (PES) (Hubbard-)satellite at around $-1.6$ eV [24,44,51]. Inverse

1The notion of locality refers to the use of a specific basis set of atom-centered orbitals, such as muffin-tin orbitals, or atom-centered Wannier functions.

2We choose a maximally localized Wannier basis [17,18] constructed separately for the correlated ($t_{2g}$) and uncorrelated subspaces, such that the one-particle Hamiltonian is block-diagonal. Then, off-block-diagonal self-energy elements are small and neglected in the following. Also, the local part of the free-energy functional then separates into correlated and uncorrelated subspace contributions. Our approach consists in calculating only the former from the impurity model, and the latter to first order in $W$.

3The GW calculation was performed for a $4 \times 4 \times 4$ $k$-point mesh, the $t_{2g}$ part of which was Wannier interpolated onto a $2^3$ mesh for the GW + DMFT self-consistency.
Figure 1(a) summarizes the LDA electronic structure: the O-p states disperse between -2 and -7 eV, separated from the t_{2g} states whose bandwidth extends from -1 eV to 1.5 eV. While the t_{2g} and e_g bands are well separated at every given k-point, the partial density of states (DOS) slightly overlap, and the e_g states display a pronounced peak at 2.3 eV. Finally, peaks stemming from the Sr-d states are located at 6.1 eV and 7.1 eV. We have superimposed to the LDA DOS the experimental PES and BIS curves taken from [44,51]. The comparison reveals the main effects of electronic correlations in this material: as expected on quite general grounds, LDA locates the filled O-p states at too high and the empty Sr-d manifold at too low energies. The t_{2g} manifold undergoes a strong quasiparticle renormalization with a concomitant shift of spectral weight to the lower Hubbard band, both of which are effects beyond the one-particle picture.

Applying the GW approximation (see the spectral function in fig. 1(b)) increases the O-p to Sr-d distance, placing both manifolds at energies nearly in agreement with experiment. Most interestingly, however, a peak at 2.6 eV emerges from the d-manifold, which we find to be of e_g character. Indeed, the GW approximation enhances the crystal field splitting and places the maximum of the e_g spectral weight at the location of the experimentally observed d^1 \rightarrow d^2 addition peak.

Also displayed is the partial t_{2g} contribution. Two interesting points are seen: the quasi-particle width is narrowed from the LDA value by about 0.5 eV and satellite structures appear below and above the Fermi level at ±3 eV, +5 eV as well as at around 15 eV. Within the (non–self-consistent) GW approximation, the self-energy is related to ImW as follows:

$$ \text{Im} \Sigma_{GW}(\epsilon_{kn} - \omega) = \sum_{k'n} \langle \psi_{kn}(r) | \text{Im} W(r',r;\epsilon_{kn} - \omega) | \psi_{k'n}^\dagger(r') \rangle. $$

Thus, a feature at \omega_0 in ImW causes a satellite feature at an energy \omega_0 below or above the quasi-particle peak at \epsilon_{kn}. In fig. 2 we display the on-site t_{2g} intra-orbital element W_{t_{2g}} of the fully screened interaction in the Wannier basis. Three notable features are clearly discernible: There is the usual high-energy electron-gas–like plasmon excitation around 15 eV and, more remarkably, there is a strong excitation between 2 and 3 eV, as well as a shoulder at ~4.5 eV. Evidently, these energy positions directly correlate with the spectral features discussed above. It is important to note that the lowest feature in W_{t_{2g}} mainly arises from a collective excitation within the t_{2g} bands. This can be understood by comparison with the Hubbard interaction U(\omega) of the low-energy t_{2g} system, as calculated within the constrained RPA. In U(\omega) the structure at 2–3 eV is absent, due to the elimination of the polarization within the t_{2g} bands. The shoulder at around 4.5 eV, a persisting slight underestimation is expected: (a) the polarization (determining W) is derived from the bare t_{2g} bands, whose character is largely too itinerant in LDA, and (b) vertex corrections are neglected.
however, partly persists, as its excitations also involve O-2p states; we will come back to this point below.

Solving the GW + DMFT equations, even without the self-consistency cycle at the GW level, that is, for fixed $\Sigma_{GW}$ and $U(\omega)$, is a hard task. We use the scheme recently introduced in ref. [4]: the Green’s function of the dynamical impurity model is obtained from a factorization ansatz $G(\tau) = G_{stat}(\tau)B(\tau)$, where $G_{stat}$ is the Green’s function of a static impurity model with constant $U = U(\omega = 0)$ (see footnote 5), and the second factor $B(\tau) = G(\tau)/G_{stat}(\tau)$ is approximated by its value for vanishing bath hybridization $\Delta$ [4]:

$$B(\tau) = \exp \left( - \int_{0}^{\infty} \frac{d\omega}{\pi} \frac{\text{Im}U(\omega)}{\omega^2} [K_{\tau}(\omega) - K_{\tau}(0)] \right)$$

with $K_{\tau}(\omega) = \exp(-\tau\omega) + \exp(-\beta - \tau\omega)$. In the regime that we are interested in, namely when the plasma frequency is several times the bandwidth, this is an excellent approximation [4].

Finally, we present our GW + DMFT results for the spectrum of SrVO$_3$ at inverse temperature $\beta = 10$ eV$^{-1}$: fig. 1(c) displays the local projection, while fig. 3 shows momentum-dependent $t_{2g}$ spectra in comparison with ARPES measurements [40,49]. The low-energy part of the spectrum is dominated by the $t_{2g}$ contribution, which, here, is profoundly modified with respect to pure GW results. A renormalized quasi-particle band disperses around the Fermi level: At the $\Gamma$-point the peak is located at about $-0.5$ eV — a strong renormalization of the corresponding Kohn-Sham state which, at this momentum, has an energy of $-1$ eV. At the $X$-point, the $t_{2g}$ bands are no longer degenerate, and surprisingly weakly renormalized $xy/xz$ states are observed at 0.9 eV, while the $yz$ band is located at nearly the same energy as at the $\Gamma$-point, in agreement with ARPES. At binding energies of 1.6 eV, ARPES witnesses a weakly dispersive Hubbard band, whose intensity varies significantly as a function of momentum [49]. In the GW + DMFT spectral function the Hubbard band — absent in GW — is correctly observed at about $-1.6$ eV, and its $k$-dependent intensity variation (see fig. 3) is indeed quite strong. Previous LDA + DMFT calculations placed the lower Hubbard band at larger negative energies (see, e.g., [28]). This is due to the fact that when using a static Hubbard interaction, a value of $4–6$ eV, that is larger than the zero frequency limit of the $ab$ initio $U(\omega = 0) = 3.6$ eV [18], is needed to account for the observed transfers of spectral weight. LDA + $U(\omega) +$ DMFT calculations taking not only the $ab$ initio value of the static component of $U$ but also its full frequency dependence into account indeed reproduce the position of the lower Hubbard band quite well [4,52]. Analogously, in GW + DMFT, the additional transfers from the dynamical screening [4,6,53], yield a good description of the Hubbard band and the spectral weight reduction at the same time.

At positive energies non-local self-energy effects are larger. Interestingly, our total spectral function, fig. 1(c), does not display a clearly separated Hubbard band. The reason is visible from the $k$-resolved spectra: the upper Hubbard band is located at around 2 eV, as expected from the location of the lower Hubbard band.
and the fact that their separation is roughly given by the zero-frequency value of $U$. The peak around 2.7 eV that appears in the inverse photoemission spectrum [51]—commonly interpreted as the upper Hubbard band of $t_{2g}$ character in the DMFT literature—arises in fact from $e_g$ states located in this energy range. The non-local self-energy effects lead, in the unoccupied part of the spectrum, to overlapping features from different $k$-points and an overall smearing of the total spectral function.

Akin to the correspondence between $\text{Im} W$ and the GW spectrum, our approach to solve the GW + DMFT equations allows for a transparent physical interpretation of the arising spectral properties. Indeed the spectral equations allows for a transparent physical interpretation of the arising spectral properties. Indeed the spectral equations allows for a transparent physical interpretation of the arising spectral properties. Indeed the spectral equations allows for a transparent physical interpretation of the arising spectral properties. Indeed the spectral equations allows for a transparent physical interpretation of the arising spectral properties. Indeed the spectral equations allows for a transparent physical interpretation of the arising spectral properties. Indeed the spectral equations allows for a transparent physical interpretation of the arising spectral properties. 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