Momentum-resolved spectral functions of SrVO₃ calculated by LDA+DMFT

I. A. Nekrasov,1,2 K. Held,3 G. Keller,2 D. E. Kondakov,4 Th. Pruschke,5 M. Kollar,2 O. K. Andersen,3 V. I. Anisimov,4 and D. Vollhardt2

1Institute for Electrophysics, Russian Academy of Sciences, Ekaterinburg 620016, Russia
2Theoretical Physics III, Centre for Electronic Correlations and Magnetism, University of Augsburg, 86135 Augsburg, Germany
3Max-Planck Institute for Solid State Research, Heisenbergstrasse 1, 70569 Stuttgart, Germany
4Institute of Metal Physics, Russian Academy of Sciences, Ekaterinburg 620219, Russia
5Institute for Theoretical Physics, University of Göttingen, Tammannstrasse 1, 37077 Göttingen, Germany

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LDA+DMFT, the merger of density functional theory in the local density approximation and dynamical mean-field theory, has been mostly employed to calculate \( k \)-integrated spectra accessible by photoemission spectroscopy. In this paper, we calculate \( k \)-resolved spectral functions by LDA+DMFT. To this end, we employ the Nth order muffin-tin (NMTO) downfolding to set up an effective low-energy Hamiltonian with three \( t_{2g} \) orbitals. This downfolded Hamiltonian is solved by DMFT yielding \( k \)-dependent spectra. Our results show a renormalized quasiparticle band over a broad energy range from −0.7 eV to +0.9 eV with small “kinks” discernible in the dispersion below the Fermi energy.

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I. INTRODUCTION

Transition metal oxides show a diversity of challenging physical phenomena, including superconductivity, metal-insulator transitions, and colossal magnetoresistance, and are therefore at the center of modern solid state research. Electrons in many of these materials are strongly correlated due to a large ratio of Coulomb interaction to bandwidth \( U/W \), resulting in complicated many-electron physics which makes realistic calculations rather difficult. In particular, conventional band structure calculations, e.g., in the local density approximation (LDA), fail because these effective one-particle approaches do not contain many-body physics such as the formation of Hubbard bands, quasiparticle renormalization, and lifetime effects. In this respect LDA+DMFT, the recent merger of LDA with the many-body dynamical mean-field theory (DMFT),5–11 is a promising new approach which includes many-body aspects into realistic calculations. It has been successfully applied, in particular to calculate the total (\( k \)-integrated) spectra of transition-metal oxides like LaTiO₃,12 V₂O₅,13–15 Sr(Ca)VO₃,15,17–22 LiV₂O₄,23 Ca₂−SrRuO₄,24,25 CrO₂,26 but also of Ni,27 Fe,28 and f-electron systems such as Pu28,29 and Ce30–35.

LDA+DMFT calculations for transition metal oxides have mostly been restricted to the \( d \) bands around the Fermi energy, employing a simplified calculational scheme based on the LDA density of states (DOS) which holds for cubic systems.3 Calculations with the full LDA Hamiltonian, including all \( spdf \) valence orbitals in the DMFT have been performed for Pu28,29 and Ce.30–33 Since the \( O_{2p} - M_{5d} \) overlap is considerable for transition metal (TM) oxides, a full LDA Hamiltonian calculation should also take into account the rather large oxygen-TM and oxygen-oxygen Coulomb interactions \( U_{pd} \) and \( U_{p} \).

While a large number of interacting orbitals makes LDA+DMFT calculations with the full \( spd \) Hamiltonian difficult, they are feasible for the effective \( d \) bands around the Fermi energy. To this end, a clear definition of the effective Hamiltonian for energies near the Fermi energy is mandatory. An accurate construction of this effective Hamiltonian is possible by the downfolding procedure for third generation muffin-tin orbitals (NMTOs) and has recently been employed in the LDA+DMFT context by Pavarini et al.19,22 Furthermore, Anisimov et al.15 recently proposed a projection scheme of the Bloch functions onto a Wannier functions basis to obtain a few-orbital Hamiltonian. Also note a third scheme, proposed by Solovyev,16 for generating Wannier functions from LMTO Bloch functions. Such a downfolded or projected Hamiltonian is required to calculate \( k \)-resolved spectra.

Due to its simple crystal structure (cubic perovskite) and the 3\( d \) electronic configuration the transition metal oxide SrVO₃ is ideal for testing new theoretical methods for the realistic modeling of correlated materials. SrVO₃ is a strongly correlated metal with a pronounced lower Hubbard band in the x-ray absorption spectrum,43 After the substitution of Sr by Ca, PES40 and Bremsstrahlung isochromat spectra44 (BIS) originally suggested the onset of a Mott-Hubbard metal-insulator transition. By contrast, thermodynamic properties (Sommerfeld coefficient, resistivity, and paramagnetic susceptibility)45 did not show significant effects upon Ca doping. An attempt to describe electronic properties of SrVO₃ by DMFT was made by Rozenberg et al.46,47 for the one-band Hubbard model using phenomenological parameters. Recently, the puzzling discrepancy between spectroscopic and thermal properties has been solved by new bulk-sensitive PES,41,42,48 showing similar spectra for CaVO₃ and SrVO₃, in agreement with the thermodynamic results. This was confirmed theoretically by LDA+DMFT calculations.15,18–22 In this paper we present LDA+DMFT (QMC) calculations for SrVO₃ based on a NMTO downfolded effective Hamiltonian for three orbitals of \( t_{2g} \).
symmetry crossing the Fermi energy. From this we calculate k-resolved spectral functions and ARPES spectra. Recently angular-resolved photoemission spectroscopy (ARPES) on SrVO$_3$ was performed, the data from Fujimori’s group allow for the direct observation of the quasiparticle mass renormalization and band edge.

The paper is organized as follows. In Sec. II we briefly discuss the crystal structure and calculate the effective $t_{2g}$ Hamiltonian for SrVO$_3$ by LDA/NMTO. In Sec. III, we discuss and compare two LDA+DMFT (QMC) calculations for SrVO$_3$, based on this effective $t_{2g}$ Hamiltonian and a simplified treatment using the DOS only. Finally, in Sec. IV the LDA+DMFT (QMC) calculated self-energy on the real axis and k-resolved spectral functions for SrVO$_3$ are presented. The paper is summarized in Sec. V.

II. CONSTRUCTION OF FEW-ORBITAL HAMILTONIANS

Starting point of a first principle calculation is usually the crystal structure. In our case, SrVO$_3$ is a perovskite with an ideal cubic $Pm\overline{3}m$ symmetry, containing one V ion in the unit cell. This implies that the main structural element, the VO$_6$ octahedron, is not distorted. The electronic configuration is 3$d^1$, which follows from the formal oxidation V$^{4+}$. Due to the cubic symmetry, the d orbitals split into two sets: three $t_{2g}$ and two $e_g$ orbitals. In our case of an octahedral coordination with oxygen, the threefold degenerated $t_{2g}$ orbitals are lower in energy than the twofold $e_g$ orbitals. Since these $t_{2g}$ and $e_g$ bands do not overlap we will later restrict our calculation to an effective Hamiltonian with three $t_{2g}$ orbitals filled with one electron per site.

For the LDA band structure calculations of SrVO$_3$, we first employed the LDA-LMTO (ASA) code version 47 which uses the basis of nonorthogonal linearized muffin-tin orbitals (LMTO; 2nd generation) in the atomic sphere approximation (ASA). Thereby, the partial waves were expanded to linear order in energy around the center of gravity of the filled part of the bands. The results are presented by thin solid lines in Fig. 1 and show 2p oxygen bands below −1.5 eV, three $t_{2g}$ bands at the Fermi energy between −1.5 eV and 1.5 eV, and $e_g$ bands between 1.5 eV and 6 eV. The other bands of our orbital basis set [O(3s, 3d), V(4s, 4p), Sr(5s, 5p, 4d, 4f)] are empty and lie far above the Fermi level.

Second, with the same basis set we employed the third generation MTO, also known as 3rd order muffin tin orbitals (NMTO). We expanded the MTOs around the three points: −2.72 eV, 0.68 eV, and 6.8 eV. Here and in the following, all energies are measured relative to the Fermi energy at 0 eV. The NMTO results are shown as dashed lines in Fig. 1 and almost coincide with LMTOs in the region of interest, i.e., O 2p and V 3d. The NMTO bands are found to be slightly lower in energy which is not surprising since third generation MTOs have the proper energy dependence in the interstitial region and, moreover, more expansion points (N + 1 = 4) for the wave function than LMTOs where N = 1 (linear approach). For the high-lying empty bands, LMTO and NMTO bands are quite different; the NMTO bands are again lower in energy. As the third NMTO expansion point (6.8 eV) is in this region, we expect NMTOs to be more precise in this region than LMTOs, which are linearized at energies corresponding to the center of gravity of the filled parts of the bands. Hence, the LMTO expansion points are below the Fermi energy, far away from these high-lying empty bands. Moreover, the second generation LMTMOs have vanishing kinetic energy in the interstitial region.

A particular advantage of NMTOs is the possibility of calculating an effective (downfolded) Hamiltonian $\hat{H}^{\text{eff}}(k)$, confined to a reduced set of orbitals in a reduced window of energies. In the case of SrVO$_3$, the $t_{2g}$ subset of the V 3d orbitals is of particular interest as discussed above. Hence, we downfolded to a 3 × 3 NMTO Hamiltonian $\hat{H}^{\text{eff}}(k)$ describing the three $t_{2g}$ orbitals. For optimizing the energy window with respect to these orbitals, we chose two NMTO expansion points, $\epsilon_1 = 0.41$ eV and $\epsilon_2 = 0.95$ eV, at the energy region of the $t_{2g}$ bands. At these energies, the NMTOs span exactly the LDA eigenfunctions. Figure 2 shows the eigenvalues of $\hat{H}^{\text{eff}}(k)$ along some high-symmetry directions in comparison with the NMTO results using the full orbital basis of Fig. 1. From the good agreement we conclude that $\hat{H}^{\text{eff}}(k)$ describes the three $t_{2g}$ bands well. The slight discrepancy at the bottom of the band could have been avoided by choosing a smaller value of $\epsilon_0$. If we increase the number of these mesh points $\epsilon$, the Hilbert space spanned by these
functions; the orthogonalization of these NMTOs will yield a slightly different representation of the LMTO method in Refs. 18 and 21, due to the oxygen 2\textsuperscript{a}hedron integration with the LMTO DOS. A minor difference to earlier calculations is that we used an orthogonalized set of orbitals, and σ the spin. \( \hat{H}_{0}^{\text{eff}} \) is a one-particle Hamiltonian generated from the LDA band structure where an averaged Coulomb interaction is subtracted to avoid double counting of the Coulomb interaction. The local intraorbital Coulomb repulsion is denoted by \( U \) and the Hund’s exchange coupling by \( J \). Rotational invariance then fixes the local interorbital Coulomb repulsion \( U' = U - 2J \), see, e.g., Ref. 54. For three orbitals, \( U' \) equals the averaged Coulomb interaction \( \bar{U} \).

The Hamiltonian (1) is then solved by the recently developed LDA+DMFT approach\(^\text{2} \) for (introductions see Refs. 3 and 6, for reviews see Refs. 4, 5, and 7). In this approach the solution of (1) is obtained by the dynamical mean-field theory (DMFT),\(^\text{9–11} \) a nonperturbative many-body method based on the \( \Delta \rightarrow \infty \) limit.\(^\text{8} \)

In this paper, \( \hat{H}_{0}^{\text{eff}} \) will be the NMTO downfolded (and symmetrically orthonormalized) Hamiltonian of Sec. II. The double counting correction is not relevant here since we consider only the three correlated \( t_{2g} \) orbitals.\(^\text{3,12} \) To calculate Coulomb interaction parameters appearing in (1) we previously\(^\text{18,21} \) employed the constrained LDA method,\(^\text{55} \) yielding an orbitally averaged Coulomb repulsion \( \bar{U} = 3.55 \) eV and a Hund’s exchange coupling \( J = 1.0 \) eV.

In our LDA+DMFT calculations, we self-consistently solve the auxiliary DMFT impurity problem\(^\text{2–11} \) by multiband quantum Monte Carlo (QMC) simulations\(^\text{56} \) together with the \( k \)-integrated Dyson equation

\[
G(\omega) = \int_{\text{BZ}} d\mathbf{k} [\omega + \mu - \Sigma(\omega)]^{-1},
\]

Here, \( G(\omega), \Sigma(\omega), \) and \( \hat{H}_{0}^{\text{eff}}(\mathbf{k}) \) are 3 × 3 matrices in orbital space, denoting the Green function, self-energy, and the downfolded NMTO Hamiltonian \( \hat{H}_{0}^{\text{eff}}(\mathbf{k}) \) in reciprocal space, respectively; \( \mu \) is the chemical potential. The simulations were done for an inverse temperature \( \beta = 10 \) eV\(^{-1} \), using 40 imaginary time slices \( (\Delta \tau = 0.25) \) and \( 2 \times 10^{5} \) Monte Carlo sweeps. Since QMC is formulated on the imaginary axis, we employed Eq. (2) for Matsubara frequencies and analytically continued \( G(\mathbf{i}\omega) \) to real frequencies by means of the maximum entropy method.\(^\text{57} \) We checked the accuracy of the calculated maximum entropy method (MEM) spectral density \( A(\omega) \) by performing ten independent self-consistent DMFT (QMC) runs, at given \( \hat{H}_{0}^{\text{eff}} \) and QMC parameters. The accuracy of the chemical potential is 0.005 eV; in the relevant energy range \( \pm 0.5 \) eV around the Fermi energy, the MEM accuracy is 0.05 eV in \( \omega \) and 2% in amplitude for \( A(\omega) \). Further away from the Fermi energy, the MEM accuracy decreases. In our previous calculations,\(^\text{18,21} \) we used a simplified scheme based on the LDA DOS only. Within a cubic symmetry, the local DMFT self-energy becomes diagonal and even orbital independent: \( \Sigma(\omega) = \delta_{\sigma\sigma'} \Sigma(\omega) \). Then, the Green functions \( G(\omega) \) of the lattice problem can be expressed via the Hilbert transform of the LDA DOS \( N(\epsilon) \)

\[
G(\omega) = \int d\epsilon \frac{N'(\epsilon)}{\omega - \mu - \epsilon - \Sigma(\omega) + i\eta},
\]

instead of Eq. (2).
In Fig. 4, we present a comparison between one-particle LDA+DMFT (QMC) spectra for SrVO₃ obtained by using Eq. (3) with the Vanadium t₂g LDA DOS (thin solid line in Fig. 3; calculated as described in Sec. II) and Eq. (2) with \( h_{\text{eff}}(k) \). Both methods give the same results, as is to be expected for a cubic system. One can see the generic “three-peak” spectrum of a strongly correlated metal: the quasiparticle peak slightly above the Fermi energy, and lower and upper Hubbard bands to the left and right. The results presented here agree well with those reported in Refs. 15 and 18–22. The LDA+DMFT calculations of Ref. 17, with a focus on bulk surface differences, used a somewhat lower Coulomb interaction \( U = U - 2J = 2.6, 2.9 \, \text{eV} \).

IV. CALCULATION OF \( k \)-RESOLVED SPECTRA

The purpose of this paper is to calculate the \( k \)-resolved spectral function \( A(k, \omega) \) for SrVO₃ within the LDA+DMFT(QMC) scheme. Here

\[
A(k, \omega) = -\frac{1}{\pi} \text{Im} \, \text{Tr} \, G(k, \omega)
\]

is determined by the diagonal elements of the Green function matrix in orbital space

\[
G(k, \omega) = \left[ \omega - \Sigma(\omega) - h_{\text{eff}}(k) \right]^{-1}.
\]

From this definition one can see that the two necessary ingredients to calculate \( A(k, \omega) \) are (i) the Hamiltonian matrix \( h_{\text{eff}}(k) \), and (ii) the self-energy matrix \( \Sigma(\omega) \) at real frequencies. Similar schemes were recently used by Liebsch and Lichtenstein to compute quasiparticle properties of Sr₃RuO₄ and by Biermann et al. to describe the presence of a lower Hubbard band in γ-Mn.

Angle-resolved photoemission spectra of the two-dimensional (2D) Hubbard model were also investigated by Maier et al. in the framework of the dynamical cluster approximation (DCA) and by Sav-dovskii et al. within the so-called DMFT+Σ₄ approach. Within DMFT the self-energy on the real axis was also calculated in Refs. 15 and 62.

In our case of cubic symmetry, \( \Sigma(\omega) \) is the same for all t₂g orbitals. Eqs. (2) and (5) are formulated in terms of a self-energy \( \Sigma(\omega) \) for real frequencies. Since LDA+DMFT (QMC) determines the self-energy \( \Sigma(i\omega_n) \) for Matsubara frequencies \( i\omega_n \), the calculation of \( \Sigma(\omega) \) requires a separate calculation. To this end we first employ the maximum entropy method to obtain the \( k \)-integrated, spectral function \( A(\omega) = -\frac{1}{\pi} \text{Im} \, G(\omega) \) with \( G(\omega) = [G(\omega)]_{\text{sym}} \) shown in Fig. 4. The Kramers-Kronig relation

\[
\text{Re} \, G(\omega) = -\frac{1}{\pi} \int_{-\infty}^{\infty} d\omega' \frac{\text{Im} \, G(\omega')}{\omega - \omega' + i\eta}
\]

then determines the real part of the Green function. The complex Green function and the complex self-energy are related by the \( k \)-integrated Dyson Eq. (2). We obtain the self-energy as the numerical solution of Eq. (2).

The unknown complex self-energy enters in the integrand of Eq. (2). After rewriting Eq. (2) as a system of two equations for the real (Re) and imaginary (Im) part of the Green function \( G(\omega) \) we solved the two equations iteratively for each energy \( \omega \). The convergence criterion was chosen as\(|\text{Re} \, \Sigma(\omega) - \text{Re} \, \Sigma_{\text{iter}}(\omega)| + |\text{Im} \, \Sigma(\omega) - \text{Im} \, \Sigma_{\text{iter}}(\omega)| < \epsilon\), where \( i \) denotes the iteration. The accuracy of the converged solution was \( \epsilon = 0.001 \, \text{eV} \) for all energy points (also see Ref. 15 Appendix B).

Figure 5 presents the resulting real and imaginary parts of the self-energy \( \Sigma(\omega) \) as a function of real frequencies. The calculated self-energy satisfies the Kramers-Kronig relation

\[
\text{Re} \, \Sigma(\omega) = -\frac{1}{\pi} \int_{-\infty}^{\infty} d\omega' \frac{\text{Im} \, \Sigma(\omega')}{\omega - \omega'} + \text{cons.}
\]
The self-energy is highly asymmetric with respect to the Fermi level, as expected for the present case of an asymmetric LDA DOS and 1/6 band filling. At the energies \( \omega \sim \pm 1.5 \text{ eV} \) the real part of the self-energy, \( \text{Re } \Sigma \), has extrema, originating from the crossover from the central quasiparticle peak to the lower and upper Hubbard bands. The two extrema of \( \text{Im } \Sigma \), which coincide with zeros of \( \text{Re } \Sigma \), are responsible for the strong incoherence of the lower and upper Hubbard bands (see Fig. 4).

Let us now turn from the Hubbard bands to the energy regime of the central (quasiparticle) peak, ranging from about \(-0.8 \text{ eV}\) to \(1.4 \text{ eV}\) in Fig. 4. The imaginary part of the self-energy \( \text{Im } \Sigma(\omega) \) is still relatively small in this regime and the real part of the self-energy can roughly be described by a straight line (dashed line in Fig. 5, main panel). This line corresponds to a quasiparticle weight \( Z=m^*/m=1-\partial \text{Re } \Sigma(\omega)/\partial \omega|_{\omega=0}=1.9 \), describing the reduction of the quasiparticle bandwidth from approximately \(3 \text{ eV}\) in LDA to \(1.5 \text{ eV}\) in LDA+DMFT. This value for \( m^*/m \) is in accord with the one determined from the lowest Matsubara frequency \( \omega_0 \), i.e., \( m^*/m=1-\frac{\text{Im } \Sigma(\omega_0)}{\omega_0}=2 \), and the estimate from the overall weight of the central (quasiparticle) peak (from \(-0.8 \text{ eV}\) to \(1.4 \text{ eV}\)): \(1/Z=m^*/m=2.2 \). It is also close to the value \( m^*/m=2.2 \) calculated in Refs. 19 and 22 and the value \( m^*/m=1.8 \pm 0.2 \) obtained in recent ARPES experiments.\(^{49} \) However, the inset of Fig. 5 reveals that, strictly speaking, the Fermi liquid regime with \( \text{Im } \Sigma(\omega) \sim \sim \omega \) and \( \text{Re } \Sigma(\omega) \sim \sim \omega \) only extends from \(-0.2 \) up to \(0.15 \text{ eV}\). In this energy range the slope of \( \text{Re } \Sigma(\omega) \) (indicated by a dashed line) is steeper than the slope of the dotted line shown in the main panel of Fig. 5. The effective mass in this low-energy regime is \( m^*_{\text{low}}/m=3 \). This is somewhat larger than the overall mass renormalization \( m^*/m=1.9 \) describing the reduction in bandwidth.

Next to this Fermi liquid regime, there are pronounced shoulders in \( \text{Re } \Sigma(\omega) \) at \( \omega=-0.25 \text{ eV} \) and \( +0.25 \text{ eV} \), with corresponding “kink”-like structures in \( \text{Im } \Sigma(\omega) \), according to the Kramers-Kronig relation (7). These shoulders of \( \text{Re } \Sigma(\omega) \) will become important in the context of the quasiparticle dispersion in Fig. 8.

Remarkably, similar “kink”-like structures on the scale of \(0.1 \text{ eV}\) below the Fermi energy were recently observed in ARPES experiment on \( \text{SrVO}_3 \) by Yoshida et al.\(^{49} \) Also note that similar structures for \( \text{Im } \Sigma(\omega) \) can be found in Ref. 62, based on LDA+DMFT (QMC) calculations for \( \text{LaTiO}_3 \).\(^{12} \) Because of the above-mentioned shoulders in \( \text{Re } \Sigma(\omega) \), \( \text{Re } \Sigma(\omega) \) can be roughly approximated by a straight line (dashed line of the main panel Fig. 5) in the overall energy regime of the central quasiparticle peak.

With the knowledge of the self-energy on the real axis, we are now in the position to calculate the \( k \)-resolved spectral functions Eqs. (4) and (5) and the quasiparticle dispersion. In Fig. 6, the LDA+DMFT (QMC) spectral functions \( A(k,\omega) \) for \( \text{SrVO}_3 \) are presented. In the energy regions \([-3 \text{ eV}, -1 \text{ eV}] \) and \([1.5 \text{ eV}, 5 \text{ eV}] \) there is some broad, non-dispersive spectral weight corresponding to the incoherent lower and upper Hubbard bands, which are hardly visible due to their almost homogeneous distribution over the whole of the Brillouin zone. Around the Fermi energy, \( A(k,\omega) \) shows a dispersive peak which is somewhat smeared out away from the Fermi energy because of lifetime effects, \( \tau^{-1} \sim \omega^2 \); Fig. 7 shows a magnification in the vicinity of the Fermi energy.

In order to calculate the spectral functions, we use the \( k \)-dependent self-energy \( \Sigma(k) \) and the effective potential \( V_{\text{eff}}(k) \). These are calculated in DMFT calculations for the one-band Hubbard model off half filling, with the numerical renormalization.

\[
G(\omega) = Z \int_{BZ} dk [\omega + Z\mu - Z\text{h}_{\text{eff}}(k)]^{-1}
\]

in the quasiparticle region. Employing this Fermi liquid behavior, and using \( 1/Z=1.9 \), we can reconstruct the band structure directly from the LDA spectrum. As seen from Fig. 8, the result (dashed curves) agrees well with the quasiparticle band (dots). However it should be noted that changes in slope of the LDA+DMFT (QMC) dispersion occur at \( \omega = -0.25 \text{ eV} \) and (hardly discernible) \( \omega = +0.25 \text{ eV} \) (see Fig. 8). These kinks stem from the shoulders in the real part of the self-energy (Fig. 5) and occur when the effective dispersion crosses over from the Fermi liquid regime with \( m^*_{\text{low}}/m=3 \) to the LDA band structure with constant renormalization \( m^*/m=1.9 \). Similar “kink”-like structures were recently found by us in DMFT calculations for the one-band Hubbard model off half filling, with the numerical renormalization.
The ratio of bandwidths yields 1/\( Z \) renormalization of the LMTO dispersion by conductors, where they have been attributed mainly to bands by 1/\( Z \) represents a simple quasiparticle renormalization of the NMTO phonons. In electronic systems kinks in the dispersion have followed their observation in various high-\( T_c \) superconductors, where they have been attributed mainly to phonons. In electronic systems kinks in the dispersion have been observed by Yoshida et al. in the ARPES spectra of SrVO\(_3\) crossing the Fermi energy. This calculation gives essentially the same kink-structured spectrum as our previous calculations based on the 2D Hubbard model within the fluctuation exchange approximation and most recently within the self-consistent projection operator method.

When comparing with experiments, we note that for \( k \)-resolved spectra the influence of PES matrix elements may be stronger than for the \( k \)-integrated spectra. Nevertheless, their inclusion affects the relative intensities but not their position. We find qualitative agreement with recent ARPES dispersions, where the renormalized band structure was observed directly. In particular, we see from Fig. 8 that the bottom of the quasiparticle band is located at approximately \( \omega = -0.7 \) eV, in contrast to the LDA value of \( \omega = -1.2 \) eV.

V. CONCLUSION

In this paper, we presented LDA+DMFT (QMC) computations of \( k \)-resolved spectral functions of SrVO\(_3\). The necessary input is an LDA-calculated Hamiltonian \( H^\text{eff}_0 \) and the LDA+DMFT self-energy at real frequencies \( \Sigma(\omega) \). We used the NMTO downfolding to calculate \( H^\text{eff}_0 \) for the strongly correlated V-\( 3d_t^2 \) orbitals of SrVO\(_3\) crossing the Fermi energy. This calculation gives essentially the same \( k \)-integrated spectrum as our previous calculations based on the 2D Hubbard model within the fluctuation exchange approximation and also been found in theoretical studies of the 2D Hubbard model within the fluctuation exchange approximation and most recently within the self-consistent projection operator method.

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Our results are in agreement with LDA calculations within the APW+lo
set of the MTO method is however more appropriate.

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