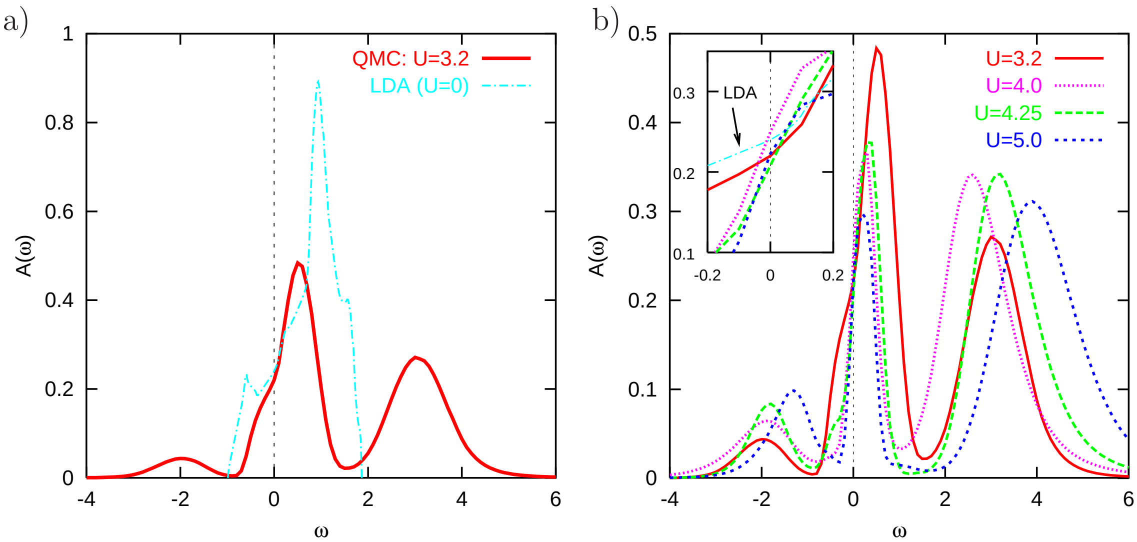

Figure 5.5: a) Partial Ti $3d$ t_{2g} LDA+DMFT(QMC) DOS for $T = 0.1$ eV and $U = 3.2$ eV in comparison to LDA. **b)** Partial Ti $3d$ t_{2g} LDA+DMFT(QMC) DOS for $T = 0.1$ for different interaction strengths. Inset: magnified view for small energies (including LDA).

following except when we discuss inverse photoemission (see Fig. 5.14).

For the solution of (5.14) for $La_{1\text{-}x}Sr_xTiO_3$ ($x = 0.06$) within the DMFT, the self-consistency equations were iterated to convergence using QMC at a relatively high temperature $k_BT = 0.1$ eV, i.e., $T \approx 1160$ K and with a discretization $\Delta\tau = 0.25\text{eV}^{-1}$. Here, the filling was fixed to $1-x$ by adjusting the chemical potential (set to 0 in the resulting spectra). Then, 40 measurements for the imaginary-time Green function $G(\tau_i)$ on the discretized grid were performed with fixed self-energy. Finally, real-time partial t_{2g} spectra were obtained using Sandvik's MEM program. As seen in Fig. 5.5 a, the explicit inclusion of a finite on-site interaction $U = 3.2$ eV changes the shape of the spectrum near the Fermi energy dramatically: in addition to the quasiparticle peak, a remnant of the noninteracting LDA DOS, lower and upper Hubbard bands appear. The spectral density $A(\omega)$ right at the Fermi energy is almost pinned to its noninteracting value, even at this comparatively high temperature. The result of corresponding calculations is shown in Fig. 5.5 b also for $U = 4$ eV, $U = 4.25$ eV, and $U = 5.0$ eV. The spread of interaction values 3.2 eV $\lesssim U \lesssim$ 5.0 eV reflects the intrinsic uncertainty in the LDA estimate for U. Clearly, the quasiparticle weight decreases with increasing U. The relatively large difference between the spectra obtained for $U = 4.0$ and $U = 4.25$ indicates significant intrinsic uncertainties which we will discuss in subsection 5.4.2.

We compare our QMC result for $U = 4.0$ with approximate solutions of the DMFT problem in Fig. 5.6 at the same temperature $T = 0.1$ eV, i.e., $T \approx 1160$ K. Most prominently, IPT misses the quasiparticle peak at this temperature since this approximation underestimates the associated Kondo temperature [cf. related observations for a three-band Hubbard model with Bethe DOS by Kajueter and Kotliar (1997)]. Moreover, the tails of the IPT spectral functions appear to have too much