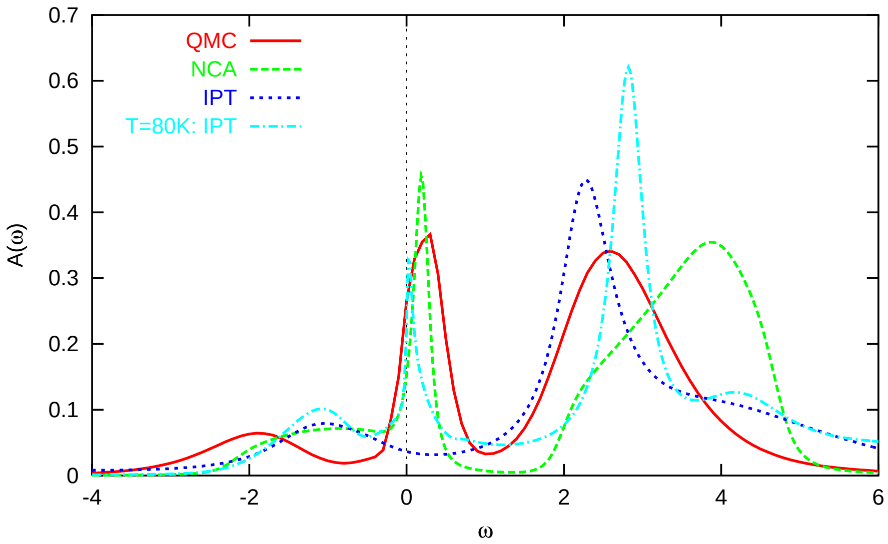

Figure 5.6: Partial Ti $3d$ t_{2g} LDA+DMFT(X) DOS for $T = 0.1$ eV and $U = 4$ eV for different approaches X for the impurity problem. Also shown is the LDA+DMFT(IPT) result for $T = 0.008$ eV.

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weight. When IPT is applied for lower temperatures $T \approx 80$ K, the quasiparticle peak is retained, but with far too small weight; the overall agreement with QMC remains fair. NCA comes off much better in comparison. However, this approximation underestimates both the weight and the width of the quasiparticle peak, cannot resolve the lower Hubbard band (but produces a shoulder too close to the quasiparticle peak instead), and shows strong deviations in the shape of the upper Hubbard band. The multi-band generalizations of NCA will usually fail at even higher temperatures than conventional NCA due to violations of proper time order in processes involving several orbitals. From the numerical comparison we conclude that the method of solution of the DMFT equations does matter.

In photoemission spectroscopy (PES), the surface of a probe is irradiated with photons of a well-defined energy above a threshold given by its work function. The intensity distribution of emitted photo electrons as a function of electron energy and angle (with energy and angle of incident photons as well as temperature, pressure etc. as parameters) is then characteristic of the material.[16] Conventionally, a distinction is made between X-ray photoemission (XPS, previously also called electron spectroscopy for chemical analysis, ESCA) and ultraviolet photoemission (UPS) depending on whether the photons originate from X-ray tubes or helium discharge lamps; more recently, however, synchrotrons provide for highly luminous sources of photons with extremely narrow energy distribution which is continuously tunable over both the XPS and UPS energy range. Within the "sudden approximation" (no

[16] While Einstein explained the photo effect in 1905 in terms of quantized radiation, i.e., photons (Nobel prize 1921), its application as an analysis tool for chemical and electronic structure of solids is due to pioneering work by Siegbahn and coworkers carried out since the fifties (Nobel prize 1981).