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Towards an ab-initio treatment of nonlocal electronic correlations with dynamical vertex approximation[1] ANNA GALLER, PATRIK GUNACKER, JAN TOMCZAK, PATRIK THUNSTRÖM, KARSTEN HELD, Vienna University of Technology — Recently, approaches such as the dynamical vertex approximation (DΓA) [1] or the dual-fermion method [2] have been developed. These diagrammatic approaches are going beyond dynamical mean field theory (DMFT) by including nonlocal electronic correlations on all length scales as well as the local DMFT correlations. Here we present our efforts to extend the DΓA methodology to ab-initio materials calculations (ab-initio DΓA) [3]. Our approach is a unifying framework which includes both GW and DMFT-type of diagrams, but also important nonlocal correlations beyond, e.g. nonlocal spin fluctuations. In our multi-band implementation we are using a worm sampling technique [4] within continuous-time quantum Monte Carlo in the hybridization expansion to obtain the DMFT vertex, from which we construct the reducible vertex function using the two particle-hole ladders. As a first application we show results for transition metal oxides. [1] A. Toschi, A. A. Katanin, and K. Held, Physical Review B 75, 045118 (2007). [2] A. N. Rubtsov, M. I. Katsnelson, A. I. Lichtenstein, Physical Review B 77, 033101 (2008). [3] A. Toschi et al., Annalen der Physik 523, 698 (2011) [4] P. Gunacker et al., Physical Review B 92, 155102 (2015)

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