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Double-counting corrections to the LDA+DMFT method in the exact density limit ANDREI VALENTIN PLAMADA, PETER STAAR, ANTON KOZHEVNIKOV, Institute for Theoretical Physics, ETH Zurich, BART YDENS, Laboratory of Solid-State Physics and Magnetism, KU Leuven, THOMAS C. SCHULTHESS, Institute for Theoretical Physics, ETH Zurich — The LDA+U method is commonly used for ab-initio studies of strongly correlated electron materials, and it has been successful in predicting spectral properties of prototypical systems such as NiO when used in conjunction with Dynamical Mean Field Theory (DMFT). Presently the method still includes an empirical term to correct doubly counted correlations. Assuming the double-counting correction is a constant μ_{DC} multiplied by the identity operator in the correlated subspace and that the electron density is well approximated with the Local Density Approximation (LDA) to Density Functional Theory, we devise a method to determine μ_{DC} directly from LDA and DMFT calculations. The method has been validated for prototypical transition metal oxides and shows promising results that agree with commonly used values for the double counting correction in the respective systems.

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