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A continued fraction approach for calculating Auger electron sprectra ANAMITRA MUKHERJEE, MONA BERCIU, GEORGE SAWATZKY, University of British Columbia — In 'core valence valence' Auger spectroscopy (AES), X-ray absorption leads to the appearance of a core hole, which then decays into two valence holes and an Auger electron. The Auger electron carries information about the spectrum of the two additional holes thus introduced in the system. This is straightforward to compute if the two holes move in an otherwise full band, but accurate results for partially filled bands are still missing. Here we present a novel approach to calculating few-body lattice Green's functions that allows us to obtain the AES spectrum for systems with both filled and open bands, such as CuO and NiO. For full bands, comparison against exact results allows us to propose efficient variational schemes, which can then be used to study partially filled bands.

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