

Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Accurate variational solution to describe a hole doped in a cuprate layer HADI EBRAHIMNEJAD, GEORGE SAWATZKY, MONA BERCIU, University of British Columbia, MONA BERCIU'S TEAM — Using a semi-analytical variational scheme, we study the spectral properties of a single hole doped in a CuO_2 plane, based on a model that includes the O 2p orbitals explicitly. We verify our choice of variational space by showing that its increase has little effect on the hole's dispersion. Our method predicts a hole dispersion that agrees very well with exact diagonalization results performed for 32-site clusters of the same model. This is quite remarkable given the much less computational effort required in our approach, which deals with an infinite lattice. We find that the low-energy states have considerable overlap with the Zhang-Rice singlet, however the overlap decreases for higher energy states, signalling the breakdown of the one-band effective treatment of this problem. Finally, we show that our results also explain the unusual drop in ARPES spectral weight observed experimentally to occur outside the magnetic Brillouin zone.

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Date submitted: 08 Nov 2013

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