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Boundary Conditions for States with Maximally Broken Time-Reversal Symmetry<sup>1</sup> ROGER HAYDOCK, C.M.M. NEX, University of Oregon — For non-crystalline materials, electronic states can only be calculated for finite clusters, and the results are sensitive to the boundary conditions. States which go to zero on the boundary have infinite life-times, appropriate for isolated clusters, but not for macroscopic materials whose states have finite life-times. Instead, we chose a boundary condition for which the states have minimal life-times, in other words, one for which the states have maximally broken time-reversal symmetry. This approach is tested for a variety of systems and compared with its close relative, the maximum entropy approximation.

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