Approximating Densities of States with Gaps using Maximally Broken Time-Reversal Symmetry[1] ROGER HAYDOCK, C.M.M. NEX, University of Oregon — When a finite cluster of atoms is used to approximate the electronic structure of a macroscopic system, the appropriate boundary condition for electronic states on the surface of the cluster is maximal flow of probability current through the boundary, or maximal breaking of time-reversal symmetry for the states. For continued fraction representations of electronic Greenians, this boundary condition gives excellent results for both the first and second sheets when there is a single band of states. In this work, the approximation is extended to Greenians for multiple bands separated by gaps, such as arise in semiconductors.

Roger Haydock
University of Oregon

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