

Abstract Submitted  
for the MAR11 Meeting of  
The American Physical Society

**Approximating Densities of States with Gaps**<sup>1</sup> ROGER HAYDOCK, C.M.M. NEX, Department of Physics and Materials Science Institute, University of Oregon — Reconstructing a density of states or similar distribution from moments or continued fractions is an important problem in calculating the electronic and vibrational structure of defective or non-crystalline solids. For single bands a quadratic boundary condition introduced previously [Phys. Rev. B 74, 205121 (2006)] produces results which compare favorably with maximum entropy and even give analytic continuations of Green functions to the unphysical sheet. In this paper, the previous boundary condition is generalized to an energy-independent condition for densities with multiple bands separated by gaps. As an example it is applied to a chain of atoms with s, p, and d bands of different widths with different gaps between them. The results are compared with maximum entropy for different levels of approximation. Generalized hypergeometric functions associated with multiple bands satisfy the new boundary condition exactly.

<sup>1</sup>Supported by the Richmond F. Snyder Fund.

Roger Haydock  
Dept. of Physics and Materials Science Institute, University of Oregon

Date submitted: 10 Nov 2010

Electronic form version 1.4