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MBTS Boundary Conditions in Continuous Systems G. A. BENESH, Department of Physics, Baylor University, ROGER HAYDOCK, Department of Physics, University of Oregon — Boundary conditions imposed on a local system that is joined to a larger substrate system often introduce unphysical reflections that affect eigenstate energies, densities of states, and charge densities. These problems are common in both atomic cluster and surface slab calculations. Solutions of the Schrodinger equation for the physical system do not possess such reflections; these wave functions carry current smoothly across the (artificial) boundary between the local system and the underlying medium. Previously, Haydock and Nex derived a non-reflecting boundary condition for discrete systems [Phys. Rev. B 75, 205121 (2006)]. Solutions satisfying this maximal breaking of time-reversal symmetry (MBTS) boundary condition carry current away from the boundary at a maximal rate—in much the same way as the exact wave functions for the physical system. The MBTS boundary condition has proved useful in discrete systems for constructing densities of states and other distributions from moments or continued fractions. The MBTS approach has now been extended to studies employing continuous spatial wave functions, including surface slab calculations and model systems. Results are compared with free slab calculations, embedding calculations, and experiment.

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