962-43-1169 Bruce R Johnson* (johnson@coral.rice.edu), Department of Chemistry, and Rice Quantum Institute, Rice University, MS 600, Houston, TX 772511892, Jeffrey L Mackey, Department of Chemistry, Rice University, MS 600, Houston, TX 772511892, and James L Kinsey, Department of Chemistry, Rice University, MS 600, Houston, TX 772511892. Solution of cartesian and curvilinear quantum equations via multiwavelets on the interval. Preliminary report.

It is shown how orthogonal compact-support multiwavelets may be used for the solution of quantum mechanical eigenvalue problems subject to specific boundary conditions. Special scaling functions and wavelets with convenient limiting behaviors at the edges of an interval are constructed in analogy to earlier work on single wavelet families. All of the integrals required for Hamiltonian matrix elements involving both regular and edge functions are calculated efficiently through use of recursion and quadrature methods. It is demonstrated through accurate eigenvalue determination that both Cartesian and curvilinear degrees of freedom are readily accommodated with such a basis, using as examples the particle in a box and the hydrogen atom in spherical polar coordinates. (Received October 02, 2000)