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The atomistic limit of envelope function theory CRAIG PRYOR, Dept. of Physics and Astronomy, University of Iowa, Iowa City, IA 52242, MATS-ERIC PISTOL, Lund University, Solid State Physics and the Nanometer structure consortium, Box 118, SE-221 00, Lund, Sweden — Electronic properties of semiconductor nanostructures and impurity states are typically calculated using one of three different methods: tight-binding models, pseudopotentials, or envelope function theory. The first two are well suited to modeling atomistic scale structures, however their parameters must be fit to bulk properties which can be a complicated procedure. In contrast, envelope function theory is best at describing larger scales in which the placement of individual atoms is not important and the parameters are directly related to experimentally determined quantities. As usually implemented, envelope function theory is insensitive to atomic scale structure. We show that this does not need to be the case, and construct an atomistic envelope function theory. This is advantageous for nanostructure modeling because it provides an atomistic model parameterized in terms of physical matrix elements rather than by complicated fitting procedures.

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