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Thermal transport in graphene nanoribbons: R-Matrix theory approach[1] K.G.S.H. GUNAWARDANA, Homer L .Dodge Department of Physics and Astronomy, Center for Semiconductor Physics in Nanostructures, The University of Oklahoma, KIERAN MULLEN, Homer L. Dodge Department of Physics and Astronomy, Center for Semiconductor Physics in Nanostructures, The University of Oklahoma — We have developed a new theoretical tool based on R-Matrix theory to calculate phonon scattering on the atomic scale. As device sizes shrink, boundary and interface scattering have become bottlenecks to thermal transport. Therefore, calculating thermal transport considering the atomistic constitution of a device is very important. In this R-Matrix approach, we consider a finite region, which is the main scattering center of the system, connected to semi-infinite leads. We develop interior region solutions (normal modes of the finite system) and lead solutions(periodic waves with dispersion) independently that can be matched at predefined boundaries to extract the transmission probabilities of each phonon modes in the lead. In this work we demonstrate the implementation of the theory for graphene nanoribbons.

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