

Abstract Submitted  
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**Quantum transport calculations using periodic boundary conditions and plane wave basis**<sup>1</sup> LIN-WANG WANG, Lawrence Berkeley National Laboratory, Berkeley, CA, 94720 — Elastic quantum transport is a fast growing research area in nanoscience. The computational method for such elastic quantum transport is still under development. Although there are many methods for transport calculations, none of them is as fast and as reliable as the conventional ground state ab initio calculations (e.g., the plane wave pseudopotential local density approximation calculation). As a result, most transport calculations are restricted to small systems. We present an efficient new method [1,2] to solve the scattering states in the quantum transport problem using periodic boundary conditions and plane wave pseudopotential method. This method allows the use of conventional ground state ab initio programs without much change, and its computational effort is similar to that of a ground state calculation. As a result, large systems containing hundreds of atoms can be calculated. Numerical results using this method for benzene molecules and doped silicon bars connected by Cu quantum wires will be presented. [1] L.W. Wang, //arxiv.org/abs/cond-mat/0408222 [2] L.W. Wang, //arxiv.org/abs/cond-mat/0408224

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