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Study of convergence in quantum transport calculations[1] JOSEPH DRISCOLL, KALMAN VARGA, Vanderbilt University Department of Physics and Astronomy — Transport calculations based on the non-equilibrium Green's function approach are most often implemented using localized atomic orbitals. We have studied the convergence properties of these calculations with respect to the number of basis states. We have found that the accuracy can be increased by using more basis states, but the computational cost rapidly increases. We show that replacing the atomic orbitals by optimized nonlocalized basis functions can significantly improve accuracy, with a lower cost than using atomic orbital states.

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