Abstract Submitted
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Computing Transport coefficients from the Microscopic Response Method[1] MINGLIANG ZHANG, DAVID A. DRABOLD, Department of Physics and Astronomy, Ohio University, Athens, Ohio 45701 — If an external perturbation to a system may be expressed as additional terms in the Hamiltonian, the microscopic response is determined by the the wave function of the system. To obtain the macroscopic response, an ensemble average can be carried out at the final stage. With the help of a systematic diagrammatic expansion, one is able to consistently compute the corresponding transport coefficient. If the spatial fluctuation of the carrier distribution is small, the microscopic response method reduces to the usual Kubo-Greenwood formula (KGF). We illustrate with the conductivity and Hall mobility of amorphous semiconductors. Because the direction of the Lorentz force is determined by the line connecting the initial and final localized states, the sign of Hall mobility in a-Si:H can be anomalous. The method is being implemented in an *ab initio* code, and it is applicable to any temperature. Thus it significantly improves upon the usual method which averages KGF over a trajectory of classical molecular dynamics.

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