Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Functional dependence of the exact time-dependent Kohn-Sham potential for quantum transport JAMES RAMSDEN, REX GODBY, University of York — We present methods for determining exact steady-state and time-dependent Kohn-Sham potentials from known charge and current densities. Applying these methods to cases of a single electron added to the conduction band of a model semiconductor, we calculate the exact Kohn-Sham potentials and discuss their meaning in the context of describing quantum transport. We show that the inclusion of a longitudinal Kohn-Sham vector potential is quite unavoidable in describing steady-state current-carrying systems, whereas the addition of an electron in a wavepacket state necessitates, inter alia, the appearance of an exchange-correlation electric field. We also present our findings on the functional dependence of the exact Kohn-Sham scalar and vector potentials on the charge and current density.

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Date submitted: 11 Nov 2011 Electronic form version 1.4