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Path integral simulations of quantized conductance in nanowires¹

JOHN SHUMWAY, Department of Physics, Arizona State University, MATTHEW GILBERT, Microelectronics Research Center, University of Texas at Austin — Theoretical studies of spin and charge transport in nanostructure often include interactions perturbatively or at a mean-field level. In some cases it is desirable to have a fully quantum many-body method to describe the interacting system: such is the case when investigating spin ordering near the “0.7-structure” in quantum point contacts or for simulating systems with strong polaronic effects. We have developed a new path-integral quantum Monte Carlo (QMC) approach to transport. Previous QMC simulations have been valued for accurately treating electronic correlation in quantum dot spectroscopy—this work now opens up many new opportunities for simulating quantum transport. We show simulation data demonstrating how current-current correlation functions in the Kubo formalism lead to quantization of conductance in GaAs nanowires. This new, finite-temperature, many-body computation technique should have many uses in the study of quantum wires and molecular electronics.

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