Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Stability of conductance oscillations in monatomic sodium wires
PETR KHOMYAKOV, GEERT BROCKS, CMS-TNW, University of Twente, P.O. Box 217, 7500 AE Enschede, The Netherlands — We study the stability of conductance oscillations in monatomic sodium wires with respect to structural variations. The geometry, the electronic structure and the electronic potential of sodium wires suspended between two sodium electrodes are obtained from self-consistent density functional theory calculations. The conductance is calculated using the Landauer-Buttiker formalism and the mode-matching technique as formulated recently in a real-space finite-difference scheme [PRB 70, 195402 (2004)]. We find a regular even-odd conductance oscillation as a function of the wire length, where wires comprising an odd number of atoms have a conductance close to the quantum unit, and even-numbered wires have a lower conductance. The conductance of odd-numbered wires is stable with respect to geometry changes in the wire or in the contacts between the wire and the electrodes; the conductance of even-numbered wires is more sensitive. Geometry changes affect the spacing and widths of the wire resonances. In the case of odd-numbered wires the transmission is on-resonance, and hardly affected by the resonance shapes, whereas for even-numbered wires the transmission is off-resonance and sensitive to the resonance shapes. Predicting the amplitude and phase of the conductance oscillation requires a first-principles calculation based upon a realistic structure of the wire and the leads.

Petr Khomyakov
CMS-TNW, University of Twente, The Netherlands

Date submitted: 17 Nov 2006 Electronic form version 1.4