

Abstract Submitted
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Ab-initio formulation of the 4-point conductance of interacting electronic systems and its implementation in the GWST method¹ PETER BOKES, Dept. of Physics, University of York, York, U.K. and Dept. of Physics, Slovak University of Technology, Bratislava, Slovakia, MATTHIEU VERSTRAETE, Dept. of Physics, University of York, York, U.K., REX GODBY, Dept. of Physics, University of York, U.K. — The commonly employed linear-response expression for the conductance of quantum junctions suffers from an ambiguity of the definition of the applied potential difference. We show how this is resolved in terms of the formally as well as physically well defined 4-point conductance [P. Bokes, J. Jung, and R. W. Godby, Phys. Rev. B 76, 125433 (2007)]. Furthermore, expressing the 4 point conductance solely in terms of the density response function or polarizability, we obtain a computationally viable approach to go beyond mean-field, Green's function based descriptions of realistic ab initio models of quantum junctions. We will discuss the numerical implementation of the formalism within the GWST code for the real-space imaginary-time GW method [N. Rojas, R.W. Godby and R.J. Needs, Phys. Rev. Lett. 74 1827 (1995)] and present results for several simple systems.

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