

Abstract Submitted
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A new expression for the conductance of quantum junctions within interacting *ab-initio* approaches¹ PETER BOKES, Department of Physics, Slovak University of Technology (FEI STU), Ilkovicova 3, 841 04 Bratislava, Slovakia, REX GODBY, Department of Physics, University of York, Heslington, York YO10 5DD, U.K. — We present a new expression for the conductance of a quantum junction [1] that is both physically appealing and numerically advantageous. First, it shows that conductance represents a strength of the Drude singularity of the conductivity $\sigma(k, k'; i\omega)$ and properly accounts for the experimental bias that results from the total field. The numerical advantage comes from the fact that instead of the current-current correlation function it is expressed in terms of density-density response which is far easier to evaluate. If formulated within time-dependent density-functional theory, it explicitly uses the exchange-correlation kernel f_{xc} or, when used within many-body perturbation theory, it makes use of the irreducible polarisation function $P(k, k'; i\omega)$. We will present its numerical implementation for a model metal-vacuum-metal interface.

[1] P. Bokes and R. W. Godby, Phys. Rev. B 69, 245420 (2004).

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