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Nonlocal Corrections to the DFT-LDA Electron Conductance in Nanoscale Systems NA SAI, University of California, San Diego, MICHAEL ZWOLAK, California Institute of Technology, GIOVANNI VIGNALE, University of Missouri-Columbia, MASSIMILIANO DI VENTRA, University of California, San Diego — Using time-dependent current-density functional theory, we derive analytically the nonlocal exchange-correlation correction to the conductance of nanoscale junctions. The correction pertains to the conductance calculated in the zero-frequency limit of time-dependent density-functional theory within the adiabatic local-density approximation. In particular, we show that in linear response the correction depends nonlinearly on the gradient of the electron density; thus, it is more pronounced for molecular junctions than for quantum point contacts. We provide specific numerical examples to illustrate these findings.

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