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Simplified Quantum Transport Theory for Finite Bias and Temperature[1] XIAOGUANG ZHANG, YUNING WU, Univ of Florida - Gainesville, SOKRATES PANTELIDES, Vanderbilt University — We reformulate the Landauer-Buttiker formula for quantum transport by explicitly accounting for the energy and bias voltage dependence of the transmission probability. Under the assumption of a constant electric field, a simple formula for the differential conductance under a finite bias and at a finite temperature is derived that does not require a nonequilibrium self-consistent calculation. Calculation for the tunneling current through Au-Benzendithiol-Au molecular junction shows excellent agreement with the nonequilibrium Green's function (NEGF) method at zero temperature. Temperature dependent I-V curves for a number of devices are demonstrated.

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