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The Third Order and the Second Order Shot Noise in Nanoscale Junctions from First Principles YU-CHANG CHEN, YU-SHEN LIU, Department of Electrophysics, National Chiao Tung University, Taiwan — We propose a field-theoretic theory allied to first principles calculations to study the third order cumulant of quantum shot noise in nanoscale junctions. Our starting point is the second-quantized field operator in terms of the effective single-particle wavefunctions obtained self-consistently within the density-functional theory. The approach is valid in both linear and nonlinear response regime and is particularly suitable in studying the third order quantum shot noise in atomic-scale junctions. As an example, we investigate the conductance, the second order shot noise, and the third order shot noises in the carbon atomic wires connected between two metal electrodes. We observe that all these physical quantities display an oscillatory behavior for even and odd number of carbon atoms.

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