

# **Numerical simulation of ballistic quantum transport in silicon nanowires accounting for full band effects**

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In ultra-scaled silicon-nanowire devices with small diameter, the transport problem can be formulated in terms of an open-boundary 1D Schrödinger equation for each subband in the longitudinal direction for electrons injected from the source and drain reservoirs. According to the equivalent Hamiltonian theorem, the kinetic operator is based on the subband energy dispersion relation  $\varepsilon(k)$  of the 1D electron gas of the nanowire, which can be accurately computed by means of an atomistic model. Even though most of the  $I$ - $V$  characteristics can be reasonably well calculated within the constant effective mass approximation, there are interesting aspects that are strictly related with the full subband structure. The numerical difficulties rising from the direct discretization of the high-order differential operator can be partly circumvented using a transfer matrix method (TMM) in combination with an expansion of  $\varepsilon(k)$  in powers of  $k^2$ . However, the TMM fails when  $\varepsilon(k)$  has relative extremes within the first Brillouin zone of the nanowire. A solution method is discussed based on the expansion of  $\varepsilon(k)$  in Fourier series, which fully accounts for the finite energy extension as well as for the periodicity of the band structure. Results will be presented relative to test potential profiles and to simulations of realistic nanowire transistors as well.