

Anton Arnold: "A hybrid WKB-based method for Schrödinger scattering problems in the semi-classical limit"

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We consider 1D scattering problems related to quantum transport in diodes. We discuss the efficient numerical integration of ODEs like $\epsilon^2 u'' + a(x)u = 0$ for $0 < \epsilon \ll 1$ on coarse grids, but still yielding accurate solutions; including oscillatory (for given $a(x) > 0$) and evanescent regimes (for $a(x) < 0$), partly including turning points. In the oscillatory case we use a marching method that is based on an analytic WKB-preprocessing of the equation. Then we shall discuss two approaches to couple the oscillatory regime to smooth regimes across turning points and close to them: In the former (evanescent) case we use a FEM with WKB-ansatz functions; in the latter case an automated switching to a Runge-Kutta method with adaptive step size controller.

Co-authors: Claudia Negulescu; Kirian Döpfner, Jannis Körner; Christian Klein, Bernhard Ujvari