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A hybrid WKB-based method for Schrödinger scattering problems in the semi-classical limit

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Abstract

We consider 1D scattering problems related to quantum transport in diodes. We discuss the efficient numerical integration of ODEs like $\varepsilon^2 u'' + a(x)\, u = 0$ for $0 < \varepsilon \ll 1$ 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.

References

[1] A. Arnold, C. Negulescu, Stationary Schrödinger equation in the semi-classical limit: numerical coupling of oscillatory and evanescent regions, *Numerische Mathematik* **138**, No. 2, 501–536 (2018).

[2] J. Körner, A. Arnold, K. Döpfner, WKB-based scheme with adaptive step size control for the Schrdinger equation in the highly oscillatory regime, *J. Comput. Appl. Math.* **404**, 113905 (2022).

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