WKB-schemes for Schrödinger-type equations

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We are concerned with the numerical integration of ODEs of the form $\epsilon^2\psi_{xx} + a(x)\psi = 0$ for given $a(x) \geq \alpha > 0$ in the highly oscillatory regime $0 < \epsilon \ll 1$ (appearing as a stationary Schrödinger equation or 1D Helmholtz equation, e.g.). In two steps we derive an accurate finite difference scheme that does not need to resolve each oscillation: 1) With a WKB-ansatz the dominant oscillations are "transformed out", yielding a much smoother ODE. 2) For the resulting oscillatory integrals we devise an asymptotic expansion both in ϵ and h. In contrast to existing strategies, the presented method has (even for a large spatial step size h) the same weak limit (in the classical limit $\epsilon \to 0$) as the continuous solution. Moreover, it has an error bound of the order $O(\epsilon^3 h^2)$. We shall give applications to k·p-Schrödinger systems and to the simulation of semiconductor-nanostructures.

REFERENCES

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