Asymptotically correct finite difference schemes for highly oscillatory linear ODEs

Jens Geier

Abstract

Numerical integration of the one-dimensional stationary Schrödinger equation $\varepsilon^2\psi(x)_{xx} + (E - V(x))\psi(x) = 0$ for a given energy $E > V_{max}$ (or related systems) can be time-consuming if $\varepsilon \ll 1$ or $E \gg V_{max}$, because of the highly oscillatory nature of the wave function. In this case, standard integrators have to use step sizes which are far smaller than the period of the solution. To decrease the numerical effort the high oscillations of the differential equation are seperated and transformed out such that the resulting system matrix is uniformly bounded with respect to the small parameter ε. The used transformation is related to the WKB-approximation of the wave function. Additionally, a numerical scheme is derived which can use a far larger step size h than the traditional schemes and has an error bound of order $\mathcal{O}(\varepsilon h^2)$.