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Numerical integrators for quantum dynamics close to the adiabatic limit. (English)

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The authors consider the numerical integration of singularly perturbed Schrödinger equations $i\dot{\psi} = \frac{1}{\varepsilon}H\psi$ where H is a time-dependent real symmetric matrix. Their goal is to develop time-reversible methods allowing for larger step sizes (in particular with $h > \varepsilon$) than traditional approaches. These methods are based on a reformulation of the equation: after a diagonalisation of H the authors introduce a new dependent variable η which represents essentially the coefficient vector of ψ with respect to an eigenbasis. This function is smoother than the original ψ and satisfies a uniform estimate on bounded time intervals. In high-dimensional problems further model reductions are possible by considering only the eigenspaces of some lower eigenvalues.

The proposed methods are similar to midpoint schemes but with an additional averaging factor. They differ in some intermediate approximation steps which are performed in a more and more complicated manner in order to obtain higher order global error estimates (which are derived rigorously in the adiabatic case). All methods require only one evaluation and diagonalisation of H per time step. They are tested and compared with other approaches at a simple model problem.

Finally, the authors discuss the problem of non-adiabatic behaviour near avoided crossings of energy levels and present an adaptive strategy for the step size reduction in such situations.

Reviewer: Werner M.Seiler (Heidelberg)

MSC:

65L05	Numerical methods for initial value problems involving ordinary differential equations
34E15	Singular perturbations for ordinary differential equations
81Q05	Closed and approximate solutions to the Schrödinger, Dirac, Klein-Gordon and other equations of quantum mechanics
34A30	Linear ordinary differential equations and systems
65L70	Error bounds for numerical methods for ordinary differential equations

Keywords:

Schrödinger equation; time-reversible integrator; adiabatic limit; quantum dynamics; singular perturbation; numerical examples; midpoint schemes; error estimates

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