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An Explicit Hermite-Taylor Method for the Schrödinger Equation

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Abstract. An explicit spectrally accurate order-adaptive Hermite-Taylor method for the Schrödinger equation is developed. Numerical experiments illustrating the properties of the method are presented. The method, which is able to use very coarse grids while still retaining high accuracy, compares favorably to an existing exponential integrator – high order summation-by-parts finite difference method.

AMS subject classifications: 65L20, 81V10

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1 Introduction

The quantum state of a physical system is described by the time dependent Schrödinger equation, which can only be solved exactly in very simplified settings. For many realistic problems the only alternative is to find approximate solutions by numerical methods. Challenges in designing numerical methods for the Schrödinger equation include: the exponential growth of the computational work with dimensionality, accurate propagation of dispersive waves and the parabolic–type time step constraint resulting form the second derivative.

For high-dimensional problems the computational cost associated with the high dimensionality can be reduced by the use of adaptive methods, especially if the solution is localized in space. To capture the dispersive properties of the solution high order accurate methods are preferred, in particular the Fourier pseudospectral method has been

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commonly used for the spatial discretization of the Schrödinger equation. Fourier based methods are spectrally accurate and capture the dispersion relation correctly, but the approximation is global making adaptive implementations all but impossible. Alternatively, high order finite difference methods, [13], which has the advantage of locality can be used. Even though high order of accuracy is easily attained in the interior of the computational domain, near the boundaries lower order accurate stencils are typically used to maintain stability. Other "method-of-lines" methods used to discretize the Schrödinger equation in space include the finite element method [9] and the Galerkin radial basis function method [10].

For most method-of-lines discretizations the parabolic time step restriction rules out the use of traditional explicit single-step and multi-step methods. Implicit single-step and multi-step methods can overcome the parabolic time step restriction but at the (often prohibitive) cost of having to solve linear systems of equations. As the equations are linear the semi-discretization takes the form of a system of first order linear ODE, $u_t = Au$, and the solution can be evolved exactly by exponentiating the matrix A. This approach is attractive as it is explicit but, being exact, does not suffer from the time step constraint. The cost of computing the matrix exponential is however large and often this type of exponential integrator method is combined with Krylov subspace methods to accelerate the computation of matrix exponential-vector products.

Aside from the absence of having to solve a large system of linear equations, required by most implicit methods, a main advantage of an explicit method is the ease of parallelization. However as previously eluded to, in order for an explicit method to be competitive it must be able to use very large cells or elements so that the parabolic time step constraint $\Delta t \leq Ch^2$, with h being a typical element size, is not overly restrictive. Local and spectrally accurate polynomial based methods such as spectral elements, discontinuous Galerkin or Hermite-Taylor methods, which are able to increase the size of the elements while increasing the polynomial degree to keep the accuracy constant, have the potential to operate in this regime. Here we develop an explicit method based on Hermite interpolation in space and evolution in time via Taylor series. This Hermite-Taylor method is spectrally accurate in space and time and, as we will show, is highly accurate on very coarse grids and with large time steps.

Hermite-Taylor methods were introduced by Hagstrom and coauthors in [5] and has since been used to solve different hyperbolic problems, see for example [1, 4] for some applications and [6] for a recent review. One of the most important features of Hermite-Taylor methods for hyperbolic problems is the ability to march the solution with a time step as large as allowed by the domain of dependence of the continuous problem. This is in stark contrast to most other polynomial based methods for hyperbolic problems, like spectral elements or discontinuous Galerkin methods. For these latter methods the time step has to be reduced by a factor of n^2 (n being the degree of the approximating polynomial) when a time- stepper with fixed order is used, and with a factor n when the order of the time-stepper is matched with the degree of the polynomials. This remarkable property of Hermite methods is rooted in the fact that Hermite methods only sample the