Abstract: The numerical approximation of the solution of the time-dependent Schrödinger equation arising in ultrafast laser dynamics is discussed. The linear Schrödinger equation is reduced to a computationally tractable, lower dimensional system of nonlinear partial differential equations by the \textit{multi-configuration time-dependent Hartree-Fock method}. This method serves to approximate the original wave function on a nonlinear manifold, using the antisymmetry inherent in the model to significantly reduce the dimension of the solution space. For the solution of the resulting systems of PDEs, several numerical techniques are compared. Space discretization using the pseudospectral method turns out to be superior to finite difference approximations. For time integration, the range of applicability and computational efficiency of high-order Runge-Kutta methods are compared with variational splitting, a method recently proposed for quantum molecular dynamics.

Key-Words: Time-dependent Schrödinger equation, multi-configuration time-dependent Hartree-Fock method, variational splitting, pseudospectral method.

1 Introduction
This paper discusses the numerical properties of a new approach to the numerical solution of the time-dependent Schrödinger equation arising in ultrafast laser dynamics.

Large-scale computations of electronic structure and dynamics pose extremely challenging problems in several areas of research. For static electronic structure computations, many different methods have been developed in various fields, such as theoretical physics or theoretical and computational chemistry. To improve on the solution of the time-independent Schrödinger equation by direct discretization, methods like \textit{density functional theory (DFT)} or \textit{(multi-configuration) Hartree-Fock (MCHF)} have been suggested.

Ultrashort strong laser pulses, however, require the solution of time-dependent initial value problems. These laser pulses developed during the last few years have opened a new regime in the interaction of fields with matter [5]. One of the most intriguing aspects is the possibility of ultrashort time-resolved spectroscopy in the sub-femtosecond time domain.

The present state of the art of numerically solving the time-dependent Schrödinger equation directly for realistic laser pulses is limited to two electron systems. The use of density functional theory for this problem is limited at least by two problems: The known approximations of the crucial “exchange correlation” term, while producing consistent ground state energies, generate contradictory and incorrect dynamical behavior and there is no applicable theory for the description of multi-electron processes, such as detachment of two electrons from an atom. While this approach promises an enormous reduction in the complexity of the computational problems, the theory is not yet developed far enough so as to be applicable to our problem, see also [4].

Therefore the present state of the art to make the original, linear Schrödinger equation tractable for numerical computation is the multi-configuration time-dependent Hartree-Fock method (MCTDHF) proposed in [8], [9], [10]. This approach produces a lower-dimensional, nonlinear system of coupled Schrödinger equations. The numerical solution of these problems is discussed in the next sections.

2 The MCTDHF Method
The model to be solved is the time-dependent Schrödinger equation for an atom or molecule with \( f \) degrees of freedom in a time-dependent electric field
In (6), only solutions $f$ \cite{8}, \cite{9}. In the case such that the ionization potential is 0.3 independent of multi-configuration time-dependent Hartree method similar to the MCTDHF approach, as compared to the arguments $x_i, \ldots, x_f$ of electrons in an atom or molecule. The Hamiltonian $H$ is time-dependent and has the form

$$
H := \sum_{k=1}^{f} \left( \frac{1}{2} (-i \nabla_k - A(t))^2 + \cdots + U(x_k) + \sum_{l \neq k} V(x_k - x_l) \right),
$$

where

$$
U(x) := - \sum_{l=1}^{f} \frac{1}{\sqrt{a^2 + (x - x_l)^2}},
$$

$$
V(x - y) := \frac{1}{\sqrt{1 + (x - y)^2}},
$$

$$
A(t) := e^{-\langle t/\tau \rangle^2 \sin(\omega t)} A_0.
$$

\nabla_k \text{ is the nabla operator w.r.t. } x_k \text{ only. For this potential, the internuclear distance is fixed at 1.4, and for each molecule the screening parameter } a \text{ is adjusted such that the ionization potential is 0.3 independent of } f \text{ \cite{8}, \cite{9}. In the case } f = 2 \text{ which we focus on in this paper, } a = 1.28 \text{ holds. Moreover, } \omega \text{ is of order of magnitude } 10^{-1}, \tau = \frac{2\pi}{\omega} n, \text{ where } n \in \mathbb{R} \text{ is of order of magnitude } 10, \text{ and } A_0 \text{ is a constant, } A_0 = O(1). \text{ For the moment, only problems in one space dimension are considered.}

In \cite{8}, \cite{9}, \cite{10}, a new approach for the approximate solution of the time-dependent Schrödinger equation is introduced: The multi-electron wave function $\psi$ from (1) is approximated by a function satisfying the ansatz

$$
\psi = \sum_{(j_1,\ldots,j_f)} \alpha_{j_1,\ldots,j_f}(t) \phi_{j_1}(x_1, t) \cdots \phi_{j_f}(x_f, t) =: \sum_J a_J \Phi_J(x, t).
$$

In (6), only solutions $\psi$ are considered which are antisymmetric under exchange of any two of their arguments $x_j, \ x_k$. This assumption is particular to the MCTDHF approach, as compared to the multi-configuration time-dependent Hartree method (MCTDH) considered, for example, in \cite{1} or \cite{6} for quantum molecular dynamics, and reduces the number of equations considerably. Particularly, the assumption implies antisymmetry in the coefficients $a_J$. Formally, multi-indices $J = (j_1,\ldots,j_f)$ vary for $j_k = 1,\ldots,N, \ k = 1,\ldots,f$. Due to the simplifications resulting from the symmetry assumption, only $C^J_N$ equations for $a_J$ have to be solved in the actual computations, however.

The Frenkel-Dirac variational principle is used to derive differential equations for the coefficients $a_J$ and the single-particle functions $\phi_k$. Thus, it is required that for $\psi$ in the manifold $\mathcal{M}$ of functions of the form of the ansatz (6),

$$
\left\langle \delta \psi \left| \frac{\partial}{\partial t} - H \right| \psi \right\rangle = 0 \quad (7)
$$

holds, where $\delta \psi$ varies in the tangent space $T_\psi \mathcal{M}$ of $\mathcal{M}$ at $\psi$.

In order to define a unique solution of (7), the additional constraints

$$
\langle \phi_j | \phi_k \rangle = \delta_{j,k}, \quad t = 0, \quad (8)
$$

$$
\langle \phi_j \left( \frac{\partial \phi_k}{\partial t} \right) \rangle = -i \langle \phi_j | g | \phi_k \rangle, \quad t \geq 0, \quad (9)
$$

are imposed, where any Hermitian operator $g$ may be used. Often, $g \equiv 0$ is chosen for reasons of simplicity, but for our numerical treatment nontrivial $g$ cannot be neglected \cite{4}. (8) together with (9) guarantees that the relation from (8) holds for all $t \geq 0$, see \cite{4}.

The variational principle (7) and the additional restrictions (8) and (9) finally yield the “working equations”

$$
i \frac{da_J}{dt} = A_H(\phi) a_J, \quad (10)
$$

$$
i \frac{\partial \Phi_J}{\partial t} = B_H(\phi) \Phi_J, \quad (11)
$$

for $a = (a_{j_1,\ldots,j_f}), \phi = (\phi_k)$. In equation (10),

$$
[A_H(\phi)]_{J,L} := \langle \Phi_J | H | \Phi_L \rangle \quad (12)
$$

is a Galerkin matrix, and (11) is derived from

$$
i \rho \frac{\partial \phi}{\partial t} = (I - P) \bar{H} \phi, \quad (13)
$$

where

$$
\psi_J := \langle \phi_J | \psi \rangle, \quad (14)
$$

$$
\rho_{j,l} := \langle \psi_j | \psi_l \rangle, \quad (15)
$$

$$
\bar{H}_{j,l} := \langle \psi_j | H | \psi_l \rangle, \quad (16)
$$
and $P$ is the orthogonal projector onto the space spanned by the functions $\phi_k$. In (14), the $L^2$ scalar product defining the single hole functions is defined with respect to the argument of $\phi_j$ only, while for the density matrix in (15) the integration is defined over all variables except one, and the mean-field operator matrix from (16) contains operators acting on one spatial variable, say $x_k$.

### 3 Numerical Methods

To solve the working equations (10) and (11) numerically, the method of lines is used. First, space discretization is applied to derive a system of ordinary differential equations. To this end, two different schemes are employed. Originally, second order finite differences on an equidistant mesh with mesh width $\Delta x$ were used to discretize the first and second derivatives in the space variable occurring in the Hamiltonian from (2) [8], i.e.,

\[
\phi_j'(x, t) \approx \frac{\phi_j(x+\Delta x, t) - \phi_j(x-\Delta x, t)}{2\Delta x},
\]

\[
\phi_j''(x, t) \approx \frac{\phi_j(x+\Delta x, t) - 2\phi_j(x, t) + \phi_j(x-\Delta x, t)}{(\Delta x)^2}
\]

for the single-particle functions $\phi_j$. This naive approximation has certain disadvantages. The approximation of the continuous Hamiltonian operator $H$ is not valid for the whole spectrum of this operator [10]: The approximation quality is $O((\Delta x)^2)$ in general, as seen in Section 4, only small eigenvalues are approximated well. Consequently, the pseudospectral method is used as a standard for space discretization. The application of the kinetic part of the Hamiltonian $H$ (which contains the derivatives w.r.t. the spatial variable) to a single-particle function $\phi_j(x, t)$ is thus approximated by

\[
(-i\nabla - A(t))^2 \approx DFT^{-1} \circ (-iD - A(t))^2 \circ DFT,
\]

where

\[
D := \text{diag}\left(\frac{k\pi}{x_{\text{end}}}\right), \quad k = -K, \ldots, K - 1.
\]

The vector of Fourier coefficients (which depend on time $t$) on an equidistant spatial grid $(x_{-K}, \ldots, x_K)$ defined on the interval $[-x_{\text{end}}, x_{\text{end}}]$ by the discrete Fourier transform $DFT$ is given by $\hat{U}(t) = (\hat{u}_{-K}(t), \ldots, \hat{u}_{K-1}(t)) = DFT(\phi_j)$, and conversely $(\phi_j(x_{-K}, t), \ldots, \phi_j(x_{K-1}, t)) = DFT^{-1}(U)$, with

\[
\hat{u}_k(t) := \frac{1}{2K} \sum_{l=-K}^{K-1} \exp\left(\frac{ik\pi x_l}{x_{\text{end}}}\right) \phi_j(x_l, t),
\]

$\hat{DFT}$ and $DFT^{-1}$ can be efficiently computed using Fast Fourier Transforms (FFT) [7].

For time integration, two methods are considered here. Most simply, the working equations (10) and (11) are solved by an explicit Runge-Kutta method, after applying either of the space discretization schemes described above. Alternatively, variational splitting is used, which was proposed in [6] for the solution of the nonlinear PDEs arising from MCTDH. In this method, the Hamiltonian $H := T + V$ from (2) is split into the parts

\[
T := \sum_{k=1}^{f} \left(\frac{1}{2}(-i\nabla_k - A(t))^2 + U(x_k)\right), \quad (17)
\]

\[
V := \sum_{k=1}^{f} \sum_{l \neq k} V(x_k - x_l). \quad (18)
\]

One step of the variational splitting method starting at $t = t_0$ with time step $\Delta t$ is defined as follows:

1. Compute $\psi_{1/2} \in M$ as the solution at time $t_0 + \frac{1}{2}\Delta t$ of

\[
\left\langle \delta \psi \left| \frac{\partial}{\partial t} - T \right| \psi \right\rangle = 0 \quad \forall \delta \psi \in T_{\psi}M, \quad (19)
\]

with initial value $\psi(t_0) = \psi_0$ (“$T$ step”).

2. Compute $\psi_{1/2}^+ \in M$ as the solution at time $t_0 + \Delta t$ of

\[
\left\langle \delta \psi \left| \frac{\partial}{\partial t} - V \right| \psi \right\rangle = 0 \quad \forall \delta \psi \in T_{\psi}M, \quad (20)
\]

with initial value $\psi(t_0) = \psi_{1/2}^-$ (“$V$ step”).

3. Compute $\psi_1 \in M$ as the solution at time $t_0 + \Delta t$ of (19) with initial value $\psi(t_0 + 1/2\Delta t) = \psi_{1/2}^+$. This symmetric splitting yields a second order approximation for the solution of the full problem (7) [6].

Now, since $T\psi \in T_{\psi}M$ for $\psi \in M \cap H^2$, the two steps of the form (19) are equivalent to solving the Schrödinger equations

\[
\frac{i}{\hbar} \frac{\partial \psi}{\partial t} = T\psi
\]

(21)
on the respective domains. If the initial function is chosen in $\mathcal{M}$, (21) decouples into a set of single particle Schrödinger equations:

$$\frac{da_j}{dt} = 0, \quad \forall J,$$

$$\frac{1}{i} \frac{\partial \phi_j}{\partial t} = \frac{1}{2} (-i \nabla - A(t))^2 \phi_j + U \phi_j, \quad \forall j. \quad (23)$$

The second splitting step (20) leads to equations

$$\frac{da}{dt} = A_V(\phi)a, \quad (24)$$

$$\frac{1}{i} \frac{\partial \phi}{\partial t} = B_V(a, \phi), \quad (25)$$

where $A_V$ and $B_V$ are defined analogously as in (10) and (11), using the operator $V$ instead of $H$.

The single particle Schrödinger equations (22) and (23) are alternatively solved by the box scheme (where the special form of the resulting system of linear equations is exploited [4]) or, more efficiently, by the pseudospectral method in conjunction with the exponential integrator for these equations is not critical, since the working equations for this case are explicitly set up in [4].

The numerical computations were performed with the MCTDHF code [10] on a Compaq SC45, where the code was compiled with the Compaq Fortran 90 Compiler V5.5.1877-48BBF.

Table 1 gives the empirical convergence orders $p$ for the solution of (10) and (11) by an explicit Runge-Kutta method of order four and for variational splitting, where finite differences are used for space discretization. $p$ is calculated from the differences in the solutions for three different step sizes $\Delta t$ in the time integration. Here, ‘err’ denotes the difference between two successive numerical approximations. The classical convergence orders four and two, respectively, are indeed retained throughout our tests, see also [3]. Since the error is monotonously decreasing, the solution computed by the Runge-Kutta method for $\Delta t = 6.25 \times 10^{-4}$ is accepted as the most accurate approximation available and used as a reference solution for the comparisons of the errors later in this section.

The main advantage of variational splitting is that the single particle Schrödinger equations and the reduced working equations can be treated independently. For (22) and (23), the discretization of the Laplacian by finite differences introduces an undesirable smoothness of the resulting ODEs. Consequently, the step size $\Delta t$ has to be chosen very small. On the other hand, (24), (25) are smoother and allow larger step sizes. It is crucial to exploit this feature, as the evaluation of the right-hand side of (25) is the computationally most expensive part of the solution algorithm. While this is not obvious for $N = f = 2$, for larger systems the computation of $B_V$ consumes the largest part of the overall run time of the program, see [3], [10]. In Table 2, the errors w.r.t. the reference solution of the numerical approximations computed by variational splitting for $\Delta t = 6.25 \times 10^{-4}$ are given, where the step sizes used for (22) and (23) are $\Delta t/2^i$, $i = 0, \ldots, 4$, and an explicit second order Runge-Kutta method is used to solve (24) and (25). Note that the integration methods proposed in [6] show a similar behavior [3]. The decrease of the step size for (22) and (23) reduces the error with or-
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<th>$p$ RK</th>
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Table 1: Convergence for Runge-Kutta method and variational splitting, space discretization by finite differences.

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Table 2: Convergence for $T$ step, variational splitting, space discretization by finite differences.

Consider two for fixed $\Delta t$ until the $T$ step is solved with the same accuracy as the $V$ step. A factor of 1/16 appears to be the optimal ratio between the two step sizes, as there is hardly any improvement in the accuracy when the step size is reduced further. With this choice of step sizes, the overall convergence order two of the method is still retained, see Table 1.

In Tables 3 and 4, the performance of the two methods is compared. Absolute and relative errors are computed w. r. t. the reference solution. In the tables, computation times (in minutes) and, more importantly, the number of evaluations of $B_V$ from (25) during the solution process is given. Note that, while the computation time for variational splitting to reach a certain level of accuracy is larger than for the Runge-Kutta method, the number of evaluations of $B_V$ is comparable or even smaller for variational splitting. This implies that for larger $N$ and $f$, variational splitting can be expected to perform well as compared to Runge-Kutta methods when finite differences are used for space discretization. Moreover, if the space discretization uses smaller $\Delta x$, Runge-Kutta methods become unstable while variational splitting is designed especially for this type of unsmoothness, see [3].

The results can be remarkably improved when the pseudospectral method is used for space discretization instead of finite differences. In addition to advantageous spectral properties of this approximation of the derivative of the solution [10], the error of the approximation decreases exponentially when the spatial grid is refined [7], while the error in the case of finite differences is $O((\Delta x)^2)$. To demonstrate this, the differences between the numerical solutions based on either discretization of the spatial derivative on grids with $K = 125, K = 250, K = 500$ and $K = 1000$ are considered, where the step size for time integration is chosen as $\Delta t = 6.25 \cdot 10^{-4}$ and the Runge-Kutta method is used. Thus a possible influence of the error introduced by time integration is eliminated. Table 5 gives the results. Indeed, it can be observed that the difference between the solutions computed using pseudospectral methods and finite differences, respectively, is $O((\Delta x)^2)$, whence it can be inferred that the pseudospectral method yields solutions with higher accuracy.

The ODEs resulting from space discretization by the pseudospectral method are apparently smoother than for finite differences. There is no advantage in choosing the step size for the $T$ step smaller than for the $V$ step. Moreover, the Runge-Kutta method performs very well in this case. To demonstrate this, the errors (again calculated w. r. t. a reference solution computed by the Runge-Kutta method with $\Delta t = 6.25 \cdot 10^{-4}$) run times and number of evaluations of the right-hand side of the differential equations are given in Tables 6 and 7. Note that in this case also, both time integration schemes show their classical convergence orders four and two, respectively, see [3]. It may be concluded...
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Table 3: Performance of Runge-Kutta method, space discretization by finite differences.

that for the equations resulting from the pseudospectral method, Runge-Kutta schemes yield more favorable results.

5 Conclusions
Numerical approximation methods for the solution of the time-dependent Schrödinger equation arising in ultrafast laser dynamics have been presented. It was demonstrated that pseudospectral methods are superior to finite difference approximations for space discretization of the nonlinear PDEs associated with the multi-configuration time-dependent Hartree-Fock method. Moreover, the potential of variational splitting methods for efficient time integration was assessed and the range of applicability and performance of the method was compared with explicit Runge-Kutta methods. It can be concluded that all the numerical methods tested work satisfactorily, and that the new methods investigated show a potential to improve the performance of standard methods. However, the best choice from among the methods tested for the numerical solution of the differential equations arising from MCTDHF is space discretization by the pseudospectral method in conjunction with time integration by explicit Runge-Kutta methods. Thus, a variable order, variable step size code based on these components is used to solve real-world problems successfully [8], [9], [10].

Acknowledgement
I am indebted to Armin Scrinzi for providing his original MCTDHF code for further development and for many discussions about the physical background, and to Wolfgang Kreuzer for implementation support.

References


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Table 4: Performance of variational splitting, space discretization by finite differences.

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Table 5: Convergence w. r. t. spatial grid, Runge-Kutta method.

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Table 6: Performance of Runge-Kutta method, space discretization by pseudospectral method.

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Table 7: Performance of variational splitting, space discretization by pseudospectral method.