An efficient parallel method for relaxing to the minimum action wavefunction

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Efficient and accurate numerical propagation of the time dependent Schrödinger equation is a problem with applications across a wide range of physics. This paper develops an efficient, trivially parallelizable method for relaxing a trial wavefunction toward a variationally optimum propagated wavefunction which minimizes the propagation error relative to a platonic wavefunction which obeys the time dependent Schrödinger equation exactly. This method is shown to be well suited for incorporation with multigrid methods, yielding rapid convergence to a minimum action solution even for Hamiltonians which are not positive definite.

As the general wave equation for nonrelativistic quantum mechanics, the time dependent Schrödinger equation holds sway over a broad range of modern physics. However, due in part to its generality, the TDSE remains a challenging problem to treat numerically. For a wavefunction expanded in a basis set, with operators represented by matrices, the wide range of physical problems described by the TDSE makes it difficult to define propagation procedures which are both general and efficient. Nearly any simplifying assumption about the form of the Hamiltonian matrix will be violated by some problem of interest, while procedures which do not make such assumptions may be computationally expensive.

The need for an efficient, general propagator for the TDSE has been highlighted in recent years by the rise of strong field physics, where problems often have particularly poor numerical properties. A typical strong field experiment may involve an electron tunneling free from a molecule due to the field of an intense laser. After reaching the continuum, the electron is accelerated by the field of the laser and may traverse hundreds of bohr before returning to scatter energetically from the parent ion. The electric field due to the laser and the continuum electron may excite the ion, while a sufficiently energetic recollision may liberate additional electrons. A strong field problem may thus include singular and irregularly shaped molecular potentials, large length scales, high energies, and time dependent, nonperturbative external forces. At present, calculations involving a single electron in three dimensions reflects a significant computational challenge, while two electron calculations may require thousands of processors.

Recently, the problem of propagating a time dependent wavefunction has been approached from the perspective of minimizing the action accumulated when the wavefunction is expanded in a particular basis. For a finite basis set, this action is not necessarily zero. Minimizing this action was shown to minimize the deviation between the propagated wavefunction and a platonic “true” wavefunction which obeys the time dependent Schrödinger equation exactly. By appropriate choice of basis set, the propagated wavefunction can be made to converge exponentially to the true wavefunction. The least action propagator thus represents a general method for accurately propagating the time dependent Schrödinger equation. However, the accuracy of this propagator is purchased at the cost of solving a potentially very large linear system of equations at every time step. For problems involving large or unstructured basis sets, where efficient propagators are most needed, direct solution of this linear system is likely to prove prohibitively expensive.

This paper addresses the problem of solving the least action linear system by developing an iterative method for decreasing the action accumulated by a trial wavefunction. By dividing a spacetime volume into many small subvolumes, the accumulated action is decreased by finding corrections which minimize the action accumulated in each subvolume. For the common case of a local Hamiltonian, corrections to the trial wavefunction in nonoverlapping subvolumes are independent of one another, making this relaxation procedure trivially parallelizable. Combining this relaxation procedure with multigrid algorithms yields an overall solution procedure which replaces the solution of a single large linear system with the solution of many small linear systems, greatly reducing the computational cost. As multigrid methods have traditionally been restricted to use with linear systems arising from elliptical PDEs, this reflects an expansion of the class of problems for which these powerful methods are suitable.

I. REVIEW OF THE LEAST ACTION PRINCIPLE

The least action propagator was derived in [3] as a way to minimize the deviation between the propagated wavefunction and a platonic “true” wavefunction which obeys the time dependent Schrödinger equation exactly. While [2] employed a Taylor series expansion for this purpose, a simpler derivation requires only the fundamental theorem of calculus. If the true wavefunction is given by \( \psi(x, t) \) and the approximate wavefunction is given by \( \phi(x, t) = \sum_{i} C_{in} \chi_{i}(\vec{x}) T_{i}(t) \), the approximation error is given by \( \delta(x, t) = \psi(x, t) - \phi(x, t) \). The norm of this deviation at some time \( t \) for a propagation step beginning
at \( t_0 \) is given by
\[
\langle \delta(t)|\delta(t) \rangle = \langle \delta(t_0)|\delta(t_0) \rangle + \int_{t_0}^{t} dt' \frac{d}{dt'} \langle \delta(t')|\delta(t') \rangle .
\] (1)

The assumption that \((i\frac{\partial}{\partial t} - H)|\psi\rangle = 0\) can be used to eliminate all terms involving \(\langle \psi|\) or \(|\psi\rangle\) from the second term, so that
\[
\langle \delta(t)|\delta(t) \rangle = \langle \delta(t_0)|\delta(t_0) \rangle - 2i \int_{t_0}^{t} dt' \langle \delta(t')|H|\delta(t') \rangle + 2i \int_{t_0}^{t} dt' \langle \phi(t')|(i\frac{d}{dt} - H)|\phi(t') \rangle .
\] (2)

In this equation, terms involving \(\phi(x,t)\) result from imperfectly propagating the wavefunction, while terms involving \(\delta(x,t)\) result from the inability to represent the true wavefunction in the chosen basis. As the propagation error is proportional to the integral of the Lagrangian density \(L = \frac{i\partial}{\partial t} - H\), the wavefunction which minimizes propagation error is that which minimizes the action accumulated over the time step.

The least action condition can be turned into a propagation scheme using the calculus of variations. For a Hamiltonian \(H = H_0 + V(x,t)\) with matrix elements in space and time given by
\[
H_{i,j} = \int dx \chi^*_i(x)H_0\chi_j(x)
\] (3)
\[
V_{ijnm} = \int_{t}^{t+\Delta t} dt' \int dx \chi^*_i(x)T_n^*(t)V(x,t)\chi_j(x)T_m(t)
\] (4)
\[
O_{i,j} = \int dx \chi^*_i(x)\chi_j(x)
\] (5)
\[
U_{n,m} = \int dt T_n^*(t)T_m(t)
\] (6)
\[
Q_{n,m} = \int dt T_n^*(t)T_m(t),
\] (7)
the action accumulated between \(t\) and \(t + \Delta t\) is given by
\[
\phi(x,t) = \sum_{i,m} C_{in}\chi_i(x)T_n(t) \text{ is given by}
\]
\[
S = \sum_{i,j,n,m} C_{in}[iO_{i,j}Q_{n,m} - H_{i,j}U_{n,m} - V_{ijnm}]C^*_{j,m}
\] (8)
and is minimized when
\[
\frac{\partial S}{\partial C^*_{j,m}} = \sum_{i,n} C_{in}[iO_{i,j}Q_{n,m} - H_{i,j}U_{n,m} - V_{ijnm}] = 0
\] (9)
for all \(j,m\). Initial and boundary conditions can be specified using Lagrange multipliers. Defining \(S' = S + \sum \lambda_i f_i^*\), where \(f_i = C_{in}T_n(t) - \langle \chi_i|x(x,t)\rangle\), minimizing \(S'\) with the constraint that \(f_i = 0\) for all \(i\) yields the minimum action solution with the initial condition \(\phi(x,t) = \sum \lambda_i |\chi_i(x)\rangle \langle \chi_i(x)|\psi(x,t)\rangle\).

When using the calculus of variations in this way, it must be remembered that it is, strictly speaking, impossible to “minimize” a complex quantity such as the action. This difficulty is particularly relevant in the context of seeking an iterative solution procedure, as the convergence of such a procedure can be more easily judged in the context of minimizing a real quantity than in approaching an extremum of a functional derivative. Accordingly, it is useful to define an action residual
\[
r_{jm} = - \sum_{i,n} C_{in}[iO_{i,j}Q_{n,m} - H_{i,j}U_{n,m} - V_{ijnm}]
\] (10)
as a quantity to measure the deviation of a wavefunction from the action-extremizing condition given by Eq. 9. Using this definition, the norm of the residual
\[
N = r_{in}O_{ij}U_{nm}r^*_{jm}
\] (11)
is positive definite, and
\[
\frac{\partial N}{\partial C^*_{j,m}} = r_{in}O_{ij}U_{nm} \frac{\partial r^*_{jm}}{\partial C^*_{j,m}} = 0
\] (12)
when the residual is zero and Eq. 9 is satisfied. Restating the least action problem in this way also gives a simple path toward improving a trial wavefunction. If a trial wavefunction gives a nonzero residual in Eq. 9, the expansion coefficients must be adjusted so as to decrease the overall norm of the action residual. Despite their technical inaccuracy, the terms “least action” and “minimizing the action” will be retained, as the terminology is familiar from classical physics.

II. ITERATIVE RELAXATION TO THE LEAST ACTION SOLUTION

The least action propagator purchases its rapid convergence to the true wavefunction at a high computational cost. For a basis with \(N_x\) spatial and \(N_t\) temporal basis functions, the least action propagator must solve for \(N_x(N_t + 1)\) coefficients (including Lagrange multipliers) at every time step. For the large and irregular spatial bases where efficient propagation schemes are most needed, the cost of directly solving the least action linear system defined by Eq. 9 is likely to prove unacceptably high.

As an alternative to direct solution, many iterative algorithms have been developed for the solution of linear systems of equations. Methods such as the conjugate gradient or generalized minimum residual algorithm attempt to solve a general linear system \(Ax = b\) by solving a smaller linear system within a Krylov subspace[4].
A common theme in such iterative methods is the need for a preconditioner $M^{-1}$ which has the effect of approximately inverting the matrix $A$. Given a trial solution \( \vec{x} \) with residual \( r = b - A\vec{x} \), a correction term \( \delta \vec{x} = M^{-1}r \) can be used to improve the trial solution, so that a new trial solution is given by \( \vec{x}' = \vec{x} + \delta \vec{x} \). In the limit that \( M^{-1} = A^{-1} \), the correction yields an exact solution; however, it is more typical to choose a preconditioner which is simple to calculate and yields acceptable performance. Generic preconditioners include Jacobi or Gauss Seidel relaxation, while physical knowledge may allow construction of preconditioners well suited to individual problems.

To define a preconditioner for the least action propagator, it is necessary to return to the action integral over a volume \( V \)

\[
S = \int dt \int_{V} d\vec{V} \phi^* L\phi, \tag{13}
\]

where \( L = i \frac{d}{dt} - H \) is the Lagrangian operator and the Hamiltonian \( H = T + V \) is the sum of a kinetic energy operator \( T = \frac{1}{2m} \nabla^2 \) and a (possibly time dependent) potential energy operator \( V \). The divergence theorem can then be used to express the kinetic energy operator in terms of singly differentiable quantities

\[
-\frac{1}{2m} \int dt \int_{V} d\vec{V} \phi^* \nabla^2 \phi = -\frac{1}{2m} \int dt \int_{\partial V} \phi^* \nabla \phi \cdot d\vec{S} + \frac{1}{2m} \int dt \int_{V} d\vec{V} \phi^* \cdot \nabla \phi \cdot d\vec{k}, \tag{14}
\]

allowing consideration of trial wavefunctions with discontinuous derivatives. Given a Lagrangian which is a local function of the spatial coordinates and some subvolume \( U \) of the original volume, the action integral can be broken up into the action accumulated inside \( U \) and that accumulated outside:

\[
S = S_U + S_{\bar{U}}, \tag{15}
\]

where

\[
S_U = -\frac{1}{2m} \int dt \int_{\partial U} \phi^* \nabla \phi \cdot d\vec{k} + \frac{1}{2m} \int dt \int_{U} d\vec{V} \phi^* \cdot \nabla \phi \cdot d\vec{k} + \int dt \int_{U} d\vec{V} \phi^* V(x,t)\phi \tag{16}
\]

and \( \bar{U} \) is the subvolume of \( V \) not contained in \( U \).

It can now be seen that the requirement that the propagated function \( \phi \) minimize the action accumulated over all space places restrictions on \( \phi_U \), the function restricted to \( U \). In order for \( \phi \) to minimize the action over all space, \( \phi_U \) must minimize the action accumulated over \( U \), subject to the requirement that \( \phi_U|_{\partial U} = \phi_{\bar{U}}|_{\partial U} \). If this were not the case, it would be possible to construct a relaxed wavefunction which would come closer to minimizing the action.

Here it is convenient to consider the norm of the least action residual. Being positive definite, this norm allows two candidate wavefunctions to be compared by the degree to which they minimize the action. Let \( N(\phi) \) be the norm of the total action residual, with \( N_U(\phi_U) \) and \( N_{\bar{U}}(\phi_{\bar{U}}) \) the norms of the action residuals inside and outside the volume of interest. If there exists some function \( \bar{\phi}_U \) for which \( N(\phi_U) > N_U(\bar{\phi}_U) \) and \( N(\bar{\phi}_U) < N_{\bar{U}}(\phi_{\bar{U}}) \), then it is possible to construct a new global wavefunction \( \phi' \), where \( \phi'_U = \phi_U \) and \( \phi'_{\bar{U}} = \bar{\phi}_U \), such that

\[
N(\phi') = N_U(\phi_U) + N_{\bar{U}}(\phi_{\bar{U}}) < N(\phi) = N_U(\phi_U) + N_{\bar{U}}(\phi_{\bar{U}}). \tag{17}
\]

This logic leads naturally to a relaxation procedure. Given a trial solution \( \phi \) and a collection of (possibly overlapping) subvolumes \( U \), the trial wavefunction may be systematically improved by minimizing the action accumulated in each subvolume, subject to the restriction that each relaxation step leave the wavefunction unchanged on the boundary and the exterior of the relaxation volume. For a local Lagrangian, relaxation over two nonoverlapping volumes is independent, allowing for parallel execution.

To cast this procedure in the form of a preconditioner, a relaxation step must find a correction \( \delta \phi \) such that \( L_U \delta \phi_U = -L_U \phi_U \), with initial conditions \( \delta \phi(x,t_0) = 0 \) and boundary conditions \( \delta \phi|_{\partial U} = 0 \).

Here it must be noted that the use of Lagrange multipliers means that the relaxed solution \( \phi + \delta \phi \) is not guaranteed to be an extremum of the action, but rather a critical point. For basis functions which are nonzero at the initial time or on the boundaries of the relaxation volume, \( \frac{\partial S}{\partial \phi} \neq 0 \), due to the nonzero Lagrange multipliers associated with imposing the boundary conditions. For this reason, the relaxation procedure described here is not guaranteed to decrease the action accumulated in the relaxation volume. As will be seen, increasing the size of the basis set within the relaxation volume helps to minimize this effect.

### III. MULTIGRID RELAXATION

The relaxation procedure introduced in the previous section has the side effect of introducing a length scale into the problem which does not originate with the PDE being solved. Because the relaxation procedure cannot change the wavefunction outside of the relaxation volume, the size of the relaxation volume affects the rate of convergence. If the space is divided up into a set of relaxation volumes of size \( \mathcal{V} \), the relaxation procedure will quickly eliminate “rough” error terms which accumulate action over volumes smaller than \( \mathcal{V} \), while error terms which accumulate action over volumes larger than \( \mathcal{V} \) will be eliminated more slowly. This problem can be rectified somewhat by relaxing over larger volumes, at the cost of increasing the size of the linear system which must be solved.
Multigrid approaches \cite{5,6} seek to eliminate this dependence on the relaxation volume by defining a treelike hierarchical basis set. At the base level, a single element is defined over the entire volume of interest. Within this element, functions are defined in terms of some small basis set – here, low order polynomials. To describe details of a function which cannot be described by this small basis set, the element is subdivided into \( n \) smaller elements, each with their own associated basis. Thus, the volume is divided into one element at the zeroth level, \( n \) elements at the first level, \( n^2 \) at the second level, and so on. This repeated subdivision produces a treelike basis, with the parents of a volume element \( e \) consisting of those elements which contain \( e \) as a subvolume and the children consisting of those elements which are a subvolume of \( e \). The leaves of the tree consist of those elements which have not been subdivided – ie, the finest level of the mesh.

In defining this treelike basis set, there is no a priori need to subdivide all volumes equally, and it may be convenient to give a compressed representation of some function by using a few coarse elements to describe the wavefunction in some region where it contains little detail, but many fine elements in some region where it oscillates more rapidly. In this way, the multigrid basis set is closely related to wavelet decomposition, and offers similar possibilities for reduction of memory and storage requirements.

The removal of the relaxation volume from the rate of convergence of the multigrid relaxation procedure is accomplished by transferring the problem between different levels of the tree, so that relaxation may occur over many different length scales. If \( P_{N}^{N-1} \) is a projection operator mapping a function defined on the \( N \)th level to a function defined on the (coarser) \( N-1 \)st level, and \( I_{N}^{N-1} \) is an interpolation operator transferring functions the other way, so that \( P_{N}^{N-1}I_{N}^{N-1} \) is the identity on the \( N-1 \)st level, and \( I_{N}^{N-1}P_{N}^{N-1} \) has eigenvalues of 1 for functions which can be expanded in the \( N-1 \)st level basis and 0 otherwise, a linear equation defined on one level can be projected onto another level. For a linear system

\[
A_N^N x^N = b^N \tag{18}
\]

defined on the fine level, the projected problem on the coarse level is given by

\[
(P_{N}^{N-1}A_{N}^N P_{N}^{T^{N-1}})(P_{N}^{N-1}x^N) = P_{N}^{N-1}b^N, \tag{19}
\]

where \( P_{N}^{T^{N-1}} = I_{N}^{N-1} \).

Given a trial solution \( \tilde{x}^N \) with residual \( r^N = b^N - A_N^N x^N \), a correction \( \delta x^N \) can be found either by solving

\[
A_N^N \delta x^N = r^N \tag{20}
\]
on the fine grid or

\[
(P_{N}^{N-1}A_{N}^N P_{N}^{T^{N-1}})(P_{N}^{N-1} \delta x^N) = P_{N}^{N-1}r^N \tag{21}
\]
on the coarse grid and interpolating to the fine grid, so that

\[
\delta x^N \approx I_{N}^{N-1}(P_{N}^{N-1}A_{N}^N P_{N}^{T^{N-1}})^{-1}P_{N}^{N-1}r^N \tag{22}
\]

The advantages of finding a correction on the coarse grid are twofold. First, there are fewer basis functions defined on the coarse grid, so that the overall problem is smaller. Second, the elements defined on the coarse grid are larger than those defined on the fine grid by a factor of \( n \), so that a relaxation scheme such as the one described in Section \[\[ \ref{section6} \] \] will eliminate error terms which accumulate in volume \( n^V \) rather than \( V \). By recursively transferring the problem between different levels of the hierarchy, error terms acquiring action over any length scale can be made to converge, ideally yielding an overall procedure which is rapidly convergent with rates of convergence which do not depend on the size of the finest element.

To date, multigrid approaches have primarily been used for problems arising from elliptical PDEs, due primarily to the lack of a suitable relaxation method to use for corrections at each level of the hierarchy. Relaxation methods such as Gauss-Seidel require a Hamiltonian which is either positive or negative definite\cite{7}. If the eigenvalue spectrum spans 0, some error terms will diverge rather than converging. For elliptical problems, convergence is guaranteed for Gauss Seidel relaxation by the positive definite Hamiltonian, while non elliptical problems such as the Schrödinger equation require that the error terms be eliminated in some other way, such as direct solution of the linear system at some level or developing an improved relaxation procedure. Multigrid approaches have been used to solve the Schrödinger equation in \[\[7\] - \[\[10\] \]. General reviews of preconditioning methods are given by \[\[11\] \[\[12\] \], while \[\[13\] \[\[14\] \] discuss preconditioners for closely related Helmholtz equation.

\section{Implementation with Legendre Polynomials}

The relaxation procedure described in this paper attempts to reduce the computational cost of performing a least action step by restricting the volume over which the action is minimized. Implicit in this restriction is the assumption that reducing the volume in this way will reduce the number of basis set coefficients to be solved for – ie, that the chosen spatial basis consists of localized basis functions which are nonzero only in a restricted range. This property is true of many popular basis sets such as finite elements or the hierarchical multigrid bases described in the previous section but not for, e.g., Gaussian basis sets of the kind commonly used in quantum chemistry. For the purposes of testing the least action relaxation procedure, a suitable basis is provided by a set of low order Legendre polynomials. The Legendre basis has the advantage that many of the matrices in the least action equation are both sparse and analytically

\[
\delta x^N \approx I_{N}^{N-1}(P_{N}^{N-1}A_{N}^N P_{N}^{T^{N-1}})^{-1}P_{N}^{N-1}r^N \tag{22}
\]
calculable, with well behaved matrix elements. In one dimension, the range $[-1,1]$ of the Legendre functions can be interpreted as a single finite element, or the interval between two grid points in the hierarchical basis. In one spatial dimension, the overlap matrices $O$ and $U$ are given by the orthogonality relation

$$\int_{-1}^{1} dy P_n(y)P_m(y) = \frac{2\delta_{nm}}{2n+1},$$

where the Q matrix is given by

$$Q_{nm} = \int_{-1}^{1} P_n'(y)P_m(y) = 2 \quad (24)$$

if $n > m$ and $\text{mod}(n-m,2) = 1$, 0 otherwise. Matrix elements of the kinetic energy operator are given by

$$T_{ij} = \frac{1}{2m} \left[ -P_i(y)P'_j(y) \right]_{-1}^{1} + \int_{-1}^{1} dy P'_i(y)P'_j(y)]$$

$$= \frac{-i(i+1) + (j^2 + j)}{2m} \quad (25)$$

when $i \neq j$ and $\text{mod}(i-j,2) = 0$, 0 otherwise. These formulas make use of the identities $P_n(1) = 1$, $P'_n(1) = \frac{n(n+1)}{2}$ and $P_n(-y) = (-1)^n P_n(y)$. For the purposes of this paper, $V_0$ is assumed to be constant throughout the volume of interest, so that matrix elements of the potential energy are proportional to the overlap matrix.

Intergrid transfer operators are constructed by subdividing the $[-1,1]$ range of the Legendre polynomials into two smaller elements, one ranging from $[-1,0]$, the other from $[0,1]$, and defining Legendre bases in the two subelements. Because $P_n \left( \frac{\alpha - 1}{2} \right)$ is an $n$th order polynomial over the range of both subelements, each basis function of the large element can be expanded as the sum of basis functions defined in the small elements, yielding interpolation matrices

$$I_{ij}^{(L)} = \int_{-1}^{1} dy' P_i \left( \frac{y' - 1}{2} \right) P_j(y')$$

for the small element on the left and

$$I_{ij}^{(R)} = \int_{-1}^{1} dy' P_i \left( \frac{y' + 1}{2} \right) P_j(y')$$

for the small element on the right, which convert from the coarse to the fine basis. Projection matrices are simply the transpose of the interpolation matrices, normalized so that $(P^{(L)} + P^{(R)}) \cdot (I^{(L)} + I^{(R)}) = I$ is the identity matrix in the parent basis.

$$P_{ij}^{(L/R)} = \frac{I_{ik}^{(L/R)}O_{kj}^{(L/R)}}{I_{ik}^{(L)}O_{kj}^{(L)}I_{ji}^{(L)} + I_{ik}^{(R)}O_{kj}^{(R)}I_{ji}^{(R)}}.$$  

In defining these matrices, the integrals of the dimensionless parameter $y$ range from $-1$ to $1$. For an element “box” of size $\Delta x\Delta t$, these integrals acquire dimension, with $I \propto 2/\Delta x$, $O_{ij} \propto \Delta x/2$, $Q_{nm} \propto 2$ and $U_{nm} \propto \Delta t/2$, and the least action equation becomes

$$C_{in}[iO_{ij}Q_{nm}\Delta x - T_{ij}U_{nm}\frac{\Delta t}{\Delta x} - O_{ij}U_{nm}V\Delta x\Delta t] = 0 \forall j, m.$$  

Defining $p_{\text{max}} = \frac{\Delta x}{\Delta t}$, this equation can be recast as

$$C_{in}[iO_{ij}Q_{nm} - 2\kappa T_{ij}U_{nm} - \nu O_{ij}U_{nm}] = 0 \forall j, m,$$  

where $\kappa = \frac{p_{\text{max}}}{\Delta t}$ is the action due to kinetic energy acquired by a particle with momentum $p_{\text{max}}$ in time $\Delta t$ and $\nu = V\Delta t$ is the action acquired due to potential energy.

Parameterizing the least action equation in this way helps to clarify the role of intergrid transfer operators in speeding convergence. If the size of the box is doubled, as might be seen in the transfer from a fine to a coarse grid, $\kappa \rightarrow \kappa/4$, while $\nu$ is unaffected. Transferring from a fine to a coarse grid is thus isomorphic to propagating for a time $\Delta t \rightarrow \Delta t/4$ in a potential $V \rightarrow 4V$. As the problem is transferred from fine to coarse grids, the kinetic energy term will disappear, while transferring from coarse to fine grids will make this term dominate. If faster convergence is needed on a grid where the potential term dominates, it may be desirable to accomplish a single timestep in two steps of size $\Delta t/2$, which will have the effect of mapping $\nu \rightarrow \nu/2$ and $\kappa \rightarrow \kappa/2$.

Because the Legendre polynomials are defined only within the confines of a single element box, it is necessary when working in the Legendre basis to enforce functional continuity at element boundaries. If $\phi^{(L)} = \sum_n C_{in}^{(L)}\chi_i^{(L)}(x)T_n(t)$ is defined in the region from $x-\Delta x$ to $x$ and $\phi^{(R)} = \sum_n C_{in}^{(R)}\chi_i^{(R)}(x)T_n(t)$ is defined in the region from $x$ to $x + \Delta x$, functional continuity is maintained by requiring that

$$\sum_i C_{in}^{(L)} = \sum_i (-1)^i C_{in}^{(R)} \forall n.$$  

Boundary and initial conditions are specified in a similar way. Requiring $\phi(x,t)$ to equal $f(x,t)$ at the initial time in some element $\alpha$ yields

$$\sum_n C_{in}^{(\alpha)}(-1)^n = \sum_n f_{in}^{(\alpha)}(-1)^n \forall \alpha, \alpha'.$$

Matching a function on the left boundary of some element $\alpha'$ yields

$$\sum_i c_{in}^{(\alpha')}(\cdot) = \sum_i f_{in}^{(\alpha')}(\cdot) \forall n,$$  

while matching the function on the right boundary of element $\alpha''$ yields

$$\sum_i c_{in}^{(\alpha'')} = \sum_i f_{in}^{(\alpha'')} \forall n.$$  

Ensuring functional continuity between element $\alpha'$ on the left and $\alpha''$ on the right yields

$$\sum_i c_{in}^{(\alpha')} = \sum_i (-1)^i c_{in}^{(\alpha'')} \forall n.$$  

(35)
When projecting a function \( f(x, t) \) into this basis, a projection which enforces continuity can be found by solving the linear system

\[
C^{(L)}_{in} + \sum_n \lambda_n = f^{(L)}_i \forall i, n \tag{36}
\]

\[
C^{(R)}_{in} + \sum_n (-1)^i \lambda_n = f^{(R)}_i \forall i, n \tag{37}
\]

\[
\sum_i C^{(L)}_{in} - \sum_i (-1)^i C^{(R)}_{in} = 0 \forall n. \tag{38}
\]

where \( f^{(\alpha)} = \int dx \int dt f(x, t) \chi^*_{i}(x)T_n(t) \) is the overlap of the basis and the expanded function over element \( \alpha \).

The least action relaxation step can be performed in one of two ways. To solve for the relaxed function directly, it is necessary to solve the least action equations with boundary conditions given by the trial wavefunction on the boundary of the relaxation volume. If \( \phi(x, t) = \sum_i C_{in} \chi_i(x)T_n(t) \) is the trial wavefunction, the relaxed wavefunction \( \phi'(x, t) = \sum_i C'_{in} \chi_i(x)T_n(t) \) is found by solving the linear system

\[
C^{(\alpha)}_{in} f^{(\alpha \beta)}_{nm} - 2\kappa T^{\alpha \beta}_{ij} U_{nm} - \nu O^{\alpha \beta}_{ij} U_{nm} = 0 \forall j, m, \beta \tag{39}
\]

with initial condition

\[
\sum_n C^{(\alpha)}_{in} (-1)^n = \sum_n C^{(\alpha)}_{in} (-1)^n \forall i, \alpha. \tag{40}
\]

boundary conditions

\[
\sum_i C^{(L)}_{in} (-1)^i = \sum_i C^{(L)}_{in} (-1)^i \forall n. \tag{41}
\]

and

\[
\sum_i C^{(R)}_{in} = \sum_i C^{(R)}_{in} \forall n. \tag{42}
\]

and internal continuity enforced by

\[
\sum_i C^{(L)}_{in} = \sum_i (-1)^i C^{(R)}_{in} \forall n. \tag{43}
\]

Alternatively, the least action linear system can be cast in the form of a correction \( \delta \phi(x, t) = \sum_i, n \delta C_{in} \chi_i(x)T_n(t) \) to a trial function \( \phi(x, t) = \sum_i, n C_{in} \chi_i(x)T_n(t) \). Let

\[
\delta C^{(\alpha)}_{in} f^{(\alpha \beta)}_{nm} - 2\kappa T^{\alpha \beta}_{ij} U_{nm} - \nu O^{\alpha \beta}_{ij} U_{nm} = 0 \forall j, m, \beta \tag{44}
\]

is the residual of the least action equations, \( \delta C^{(\alpha)}_{in} \) can be found by solving

\[
\delta C^{(\alpha)}_{in} f^{(\alpha \beta)}_{nm} = \tau_{jm} \forall j, m, \beta \tag{45}
\]

with initial condition

\[
\sum_n \delta C^{(\alpha)}_{in} (-1)^n = 0 \forall i, \alpha. \tag{46}
\]

boundary conditions

\[
\sum_i \delta C^{(L)}_{in} (-1)^i = 0 \forall n, \tag{47}
\]

and

\[
\sum_i \delta C^{(R)}_{in} = 0 \forall n, \tag{48}
\]

and internal continuity enforced by

\[
\sum_i \delta C^{(L)}_{in} = \sum_i (-1)^i \delta C^{(R)}_{in} \forall n. \tag{49}
\]

Restating the problem in the form of solving for a correction to a trial wavefunction has the additional advantage that all terms in the least action linear system can be acted upon by intergrid transfer operators, making the problem susceptible to multigrid approaches.

V. CONVERGENCE

The relaxation procedure described in this paper seeks to solve for the minimum action wavefunction for a given initial condition by iteratively decreasing the action accumulated by a series of trial wavefunctions. Convergence to the true minimum action wavefunction is achieved when the action can no longer be lowered, and the residual of the least action equation is zero.

The convergence of the relaxed wavefunction to the minimum action solution was tested by expanding a trial wavefunction of the form \( f(x, t) = e^{i(kx + \omega t)} \) into a Legendre basis consisting of either one element ranging from \([-1, 1]\) or two elements ranging from \([-1, 0]\) and \([0, 1]\). Convergence was measured by taking the ratio of the magnitude of the accumulated action before and after relaxation, or alternatively by taking the ratio of the norm of the action residuals. Rates of convergence using one element are shown in Figures 1 and 2, while rates of convergence using two elements are shown in Figures 3 and 4. Because \( \kappa \) and \( \nu \) may vary widely from problem to problem, or within the same problem due to intergrid transfer, calculations were made for a wide range of both parameters, including \( \kappa >> 1 \), corresponding to large amounts of action due to high kinetic energy, and \( \nu < 0 \), where the energy eigenvalue spectrum spanned zero. For all values of \( \kappa \) and \( \nu \) tested, the relaxation procedure yielded rapid rates of convergence in the limit of sufficiently large basis sets. Rates of convergence were somewhat higher for calculations made with larger basis sets, although this must be balanced against the higher cost of an individual relaxation step. More important was the requirement that the basis set yield sufficient free parameters to allow for convergence while satisfying \( N_x + N_t (2 + N_x - 1) \) constraint equations, where \( N_x \) is the number of elements. For \( N_x = N_t = 3 \) the 9 free parameters are matched by 9 constraint equations for a single element calculation.
while a two element calculation yields 18 free parameters and 12 constraints. The large number of constraint equations, with corresponding action costs in the form of Lagrange multipliers, means that rates of convergence may be slow or even diverging for small basis sets. Higher order basis sets yielded rapid convergence over nearly all of parameter space, with convergence slowing only in the vicinity of the \(w = 1/2 + \nu\) curve where the trial solution is already a good approximation to the minimum action wavefunction.

Comparing these figures, it is apparent that relaxing over two elements simultaneously is very inefficient. As the cost of solving a linear system for \(n\) unknowns scales as \(n^3\), relaxing over 2 volumes simultaneously is approximately 4 times as expensive as relaxing over each volume separately. However, comparing figures 1 and 3 or 2 and 4 shows that this added expense does not result in appreciably faster rates of convergence. Despite this inefficiency, the inability of the relaxation procedure to change the wavefunction on the boundary of the relaxation volume means that a convergent procedure must at some point relax over volumes larger than a single element.

A more efficient way of relaxing over large volumes makes use of intergrid transfer operators. In Figures 5 and 6, relaxation over two adjacent volumes was accomplished by first transferring the residual from two fine elements to one coarse element using Eq. [21]. The correction found on the coarse grid was then transferred back to the fine grid using Eq. [22]. This partially relaxed wavefunction was then relaxed over the two fine elements separately. In all, this process involved solving 3 linear systems of size \(n\), so that the computational effort was 1.5 times that of relaxing over each volume separately. However, comparing figures 1 and 3 or 2 and 4, relaxing over both volumes at once. The decrease in computational effort is more pronounced in higher dimensions: using intergrid transfer to relax over a hypercube of \(2^d\) elements increases costs by a factor of \(1 + 2^d\) relative to relaxing over each element separately, while relaxing over the entire hypercube simultaneously increases costs by a factor of \(2^{2d}\).

VI. CONCLUSIONS

Efficiently and accurately propagating a time dependent wavefunction is a fundamental problem of computational quantum mechanics, with applications ranging across many areas of physics. This paper has addressed this problem by developing an iterative procedure for relaxing a trial wavefunction toward a variationally optimum, action minimizing solution. This relaxation procedure is trivially parallelizable for problems involving a local Hamiltonian, and does not rely on the Hamiltonian being positive definite, making it well suited for incorporation into multigrid relaxation methods. A local Fourier analysis shows that this procedure yields rapid rates of convergence over a wide range of parameters in the limit that the basis set defined over a particular volume element is sufficiently large.

Although the discussion in this paper has focused on the specific problem of the time dependent Schrödinger equation, the analysis depends primarily on the existence of a local Hamiltonian. As this is a very common condition in physical problems, it may in the future be desirable to extend this analysis to other computationally difficult problems.

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FIG. 2. (Color online) Log ratio of the magnitude of the accumulated action before and after relaxation vs wavenumber (horizontal) and frequency (vertical) for trial wavefunction $f(x, t) = e^{i(kx + \omega t)}$, calculated using a single volume element. Columns show convergence for a given number of spatial and temporal basis functions, while rows show convergence for different values of the parameters $\kappa$ and $\nu$ in Eq. 30. a) $\kappa = 0$, $\nu = 0$, b) $\kappa = 0.1$, $\nu = 0$, c) $\kappa = 1.0$, $\nu = 0$, d) $\kappa = 10.0$, $\nu = 0$, e) $\kappa = 0$, $\nu = 1.0$, f) $\kappa = 0$, $\nu = -1.0$, g) $\kappa = 1.0$, $\nu = 1.0$, h) $\kappa = 1.0$, $\nu = -1.0$. Red areas correspond to ratios greater than 1.0, where the relaxation procedure does not converge.
FIG. 3. (Color online) Log ratio of the residual norm before and after relaxation vs wavenumber (horizontal) and frequency (vertical) for trial wavefunction $f(x, t) = e^{i(k x + \omega t)}$, calculated using two adjacent volume elements. Columns show convergence for a given number of spatial and temporal basis functions, while rows show convergence for different values of the parameters $\kappa$ and $\nu$ in Eq. 30: a) $\kappa = 0$, $\nu = 0$, b) $\kappa = 0.1$, $\nu = 0$, c) $\kappa = 1.0$, $\nu = 0$, d) $\kappa = 10.0$, $\nu = 0$, e) $\kappa = 0$, $\nu = 1.0$, f) $\kappa = 0$, $\nu = -1.0$, g) $\kappa = 1.0$, $\nu = 1.0$, h) $\kappa = 1.0$, $\nu = -1.0$. Red areas correspond to ratios greater than 1.0, where the relaxation procedure does not converge.
FIG. 4. (Color online) Log ratio of the magnitude of the accumulated action before and after relaxation vs wavenumber (horizontal) and frequency (vertical) for trial wavefunction $f(x,t) = e^{i(kx+\omega t)}$, calculated using a two adjacent volume elements. Columns show convergence for a given number of spatial and temporal basis functions, while rows show convergence for different values of the parameters $\kappa$ and $\nu$ in Eq. 30: a) $\kappa = 0$, $\nu = 0$, b) $\kappa = 0.1$, $\nu = 0$, c) $\kappa = 1.0$, $\nu = 0$, d) $\kappa = 10.0$, $\nu = 0$, e) $\kappa = 0$, $\nu = 1.0$, f) $\kappa = 0$, $\nu = -1.0$, g) $\kappa = 1.0$, $\nu = 1.0$, h) $\kappa = 1.0$, $\nu = -1.0$. Red areas correspond to ratios greater than 1.0, where the relaxation procedure does not converge.
FIG. 5. (Color online) Log ratio of the residual norm before and after relaxation vs wavenumber (horizontal) and frequency (vertical) for trial wavefunction \( f(x, t) = e^{i(kx + \omega t)} \), calculated for two adjacent elements using the intergrid transfer method. Columns show convergence for a given number of spatial and temporal basis functions, while rows show convergence for different values of the parameters \( \kappa \) and \( \nu \) in Eq. 30.

- a) \( \kappa = 0, \nu = 0 \)
- b) \( \kappa = 0.1, \nu = 0 \)
- c) \( \kappa = 1.0, \nu = 0 \)
- d) \( \kappa = 10.0, \nu = 0 \)
- e) \( \kappa = 0, \nu = 1.0 \)
- f) \( \kappa = 0, \nu = -1.0 \)
- g) \( \kappa = 1.0, \nu = 1.0 \)
- h) \( \kappa = 1.0, \nu = -1.0 \)

Red areas correspond to ratios greater than 1.0, where the relaxation procedure does not converge.
FIG. 6. (Color online) Log ratio of the magnitude of the accumulated action before and after relaxation vs wavenumber (horizontal) and frequency (vertical) for trial wavefunction $f(x, t) = e^{i(kx + \omega t)}$, calculated for two adjacent elements using the intergrid transfer method. Columns show convergence for a given number of spatial and temporal basis functions, while rows show convergence for different values of the parameters $\kappa$ and $\nu$ in Eq. 30. a) $\kappa = 0, \nu = 0$, b) $\kappa = 0.1, \nu = 0$, c) $\kappa = 1.0, \nu = 0$, d) $\kappa = 10.0, \nu = 0$, e) $\kappa = 0, \nu = 1.0$, f) $\kappa = 0, \nu = -1.0$, g) $\kappa = 1.0, \nu = 1.0$, h) $\kappa = 1.0, \nu = -1.0$. Red areas correspond to ratios greater than 1.0, where the relaxation procedure does not converge.