Adaptive potential in alternating-direction implicit relaxation

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Abstract

We demonstrate a useful decomposition of the potential energy, which accelerates the relaxation method for finding the ground state of a Schrödinger operator in multiple space dimensions, and improves the ultimate accuracy achievable. The potential decomposition makes the Schrödinger operator approximately separable for the evolving approximation to the ground state; this decreases the error associated with the long time-steps in alternating-difference implicit schemes.

I. Review and Motivation

A central step in many quantum modeling problems is to find the lowest-energy eigenstates of a Hamiltonian operator. A standard approach to find them is the relaxation technique [1].

The relaxation technique, applied to find the ground state of Hamiltonian H, amounts to evolution of the Schrödinger equation in imaginary time:

$$H\varphi(t) = -\hbar\, \partial_t \varphi(t)\,, \tag{1}$$

Starting from an initial condition that has nonzero overlap with the ground state, the ground state is asymptotically dominant after imaginary times long compared to $\tau_{10} \equiv \hbar/(E_1 - E_0)$,

$$\varphi(t) \sim a_0(t)\, \varphi_0\,. \tag{2}$$

(E_0 and E_1 are the ground and first excited energies of the Hamiltonian, respectively; a_0 is a space-independent coefficient.) The primary goals in such an evolution are stability and accuracy. Implicit techniques exist which are well-known to yield stable evolution both in real and imaginary time, in which accuracy can always be assured by using a sufficiently small time step Δt. The simplest of these is

$$\left(1 + \Delta t H/\hbar \right) \varphi^j = \varphi^{j-1}\,, \tag{3}$$

with $\varphi^j \equiv \varphi(t_j)$; $t_j = j\Delta t$.

However, just as not all eigenstates are required, similarly not every kind of accuracy is required either. In particular, since the object of the relaxation is simply to remove the high-energy components as rapidly as possible, in order to examine what is left, an accurately exponential decay of those components is less important than their mere rapid disappearance.

For this reason, it is common to accelerate the relaxation procedure by using long time steps. When this acceleration is used with one-dimensional Hamiltonians, one converges to the ground state.

The evolution described in (3), like other implicit evolution methods, requires inversion of a large matrix (in this case, the matrix representing $1 + \Delta t\, H/\hbar$). The matrix to be inverted has a dimension equal to the number mesh points. This dimension grows as the inverse of the mesh

spacing raised to the power of the mesh dimension. For multidimensional problems, this inversion is impractical or numerically intractable. Instead, standard time-evolution techniques for multi-dimensional Hamiltonians typically use an operator-separation or alternating-direction implicit (ADI) scheme. For example, decomposing a two-dimensional Hamiltonian H^{2D} as

$$H^{2D} = H^x + H^y , \tag{4}$$

one may write

$$\varphi^j = \frac{1}{1 + \Delta t\, H^x/\hbar} \; \frac{1}{1 + \Delta t\, H^y/\hbar} \; \varphi^{j-1} , \tag{5}$$

or equivalently:

$$\left(1 + \Delta t\, H^y/\hbar\right) \varphi^{j-0.5} = \varphi^{j-1} , \tag{6a}$$

$$\left(1 + \Delta t\, H^x/\hbar\right) \varphi^{j} = \varphi^{j-0.5} . \tag{6b}$$

If H^x and H^y involve only the kinetic energy of motion along x and y directions respectively, then each step (6a, 6b) requires the solution only of a tridiagonal matrix.

In ADI schemes, short time steps are necessary not only for the accurate exponential decay of high-energy states, *but also for the accurate estimation of the ground state.* For example, in (5), φ approaches the ground state of

$$H' \equiv H^{2D} + H^x H^y \frac{\Delta t}{\hbar} , \tag{7}$$

which by perturbation theory implies a ground state energy that also is accurate only to first order in Δt. As a result, while short time steps may be used initially to accelerate the dissipation of high-energy components, eventually short time steps must be used to achieve accurate ground states. In this kind of variable time-step relaxation, it can be difficult to determine unambiguously how well one is converging. (See however, work by Doss and Miller on ADI solution of Laplace and related equations [2], in which a way is found to optimize the time step.) In general, efficient use of this approach can require a certain amount of user interaction, and is correspondingly difficult to program for systematic application.

Separable Hamiltonians constitute an important exception to the above distinction between one-dimensional and higher-dimensional. That is, if an ADI scheme consists of the alternating application of the separated components of a separable Hamiltonian, then relaxation converges to the appropriate ground state even for large time steps. [This can be seen immediately in (7), from the fact that the ground state is simultaneously an eigenstate of H^x and H^y as well as H^{2D}.] Most Hamiltonians (almost all, in the appropriate probability-measure sense) cannot be put into separable form. However, as we describe below, it *is* possible to find a decomposition that is separable in a restricted sense: the Hamiltonian is partitioned in such a way that at least the ground state is simultaneously an eigenstate of each partitioned component. This permits an acceleration of relaxation without the usual penalty in accuracy.

II. Adaptive Potential

Most Hamiltonians (almost all, in the appropriate probability-measure sense) cannot be put into separable form. However, as we describe below, it *is* possible to find a decomposition that is separable in a restricted sense, thus permitting an acceleration of relaxation without the usual penalty in accuracy.

In order to simplify the presentation, we here consider only two-dimensional Hamiltonians (4). We seek new potentials $V_0^x(x,y)$ and $V_0^y(x,y)$ so that, with

$$H_0^x = K^x + V_0^x \quad , \quad H_0^y = K^y + V_0^y \, , \tag{8}$$

the ground state φ_0 of H^{2D} also satisfies the auxiliary equations

$$H_0^x \varphi_0 = H_0^y \varphi_0 = \tfrac{1}{2} E_0 \, \varphi_0 \, . \tag{9}$$

If φ_0 is known, (9) can be solved for the potentials using (8). Because the total potential must always be V, it suffices to determine only the single function

$$\Delta V \equiv \frac{1}{2}\left(V^x - V^y\right) . \tag{10}$$

During the time evolution, one knows only φ, the evolving best approximation to φ_0. To indicate this we omit the zero subscripts on the separated potentials. Assuming that $\varphi - \varphi_0$ small, we "solve" (9) to find

$$\Delta V[\varphi] = -\frac{(K^x - K^y)\varphi}{2\varphi} \tag{11}$$

In the adaptive-potential ADI (APADI) approach, we recompute ΔV after each time step. Using this ΔV directly to define the current potential is unstable, so instead we relax exponentially toward the instantaneous potential, with ΔV for the ith time step defined by:

$$\Delta V^i \equiv (1-\alpha)\Delta V^{i-1} + \alpha \, \Delta V[\varphi^{i-1}] \, , \tag{12}$$

and depending on a relaxation parameter α.

III. Numerical Results

We have applied the potential (12) in both first-order and second-order operator separation schemes. We first treat a separable example (a sum of finite square-well potentials, in the x and y directions) in order to compare the adaptive-potential ADI (APADI) scheme not only with naïve-potential ADI (NPADI: $V^x = V^y = V/2$) but also with the a partition using the exact separated potentials ADI (SPADI). Figure 1 compares these in a first-order scheme. We plot the fractional deviation of the computed ground state energy from the exact ground-state energy, using a constant time step ($\Delta t = 2$, in units chosen so that the electron mass, ångström, and electron-volt have unit magnitude), with a one-dimensional well depth of 0.2 eV, a well-width of 40 Å, and electron mass of 0.1 × free-electron mass. The relaxation parameter α is 0.05. APADI clearly represents a significant improvement over the standard approach, represented by NPADI.

After $t \approx 200$, SPADI fluctuates due to round-off error. Using second-order operator separation ("true" ADI), the APADI scheme is significantly better, to the extent that APADI and SPADI differ only in this round-off error regime.

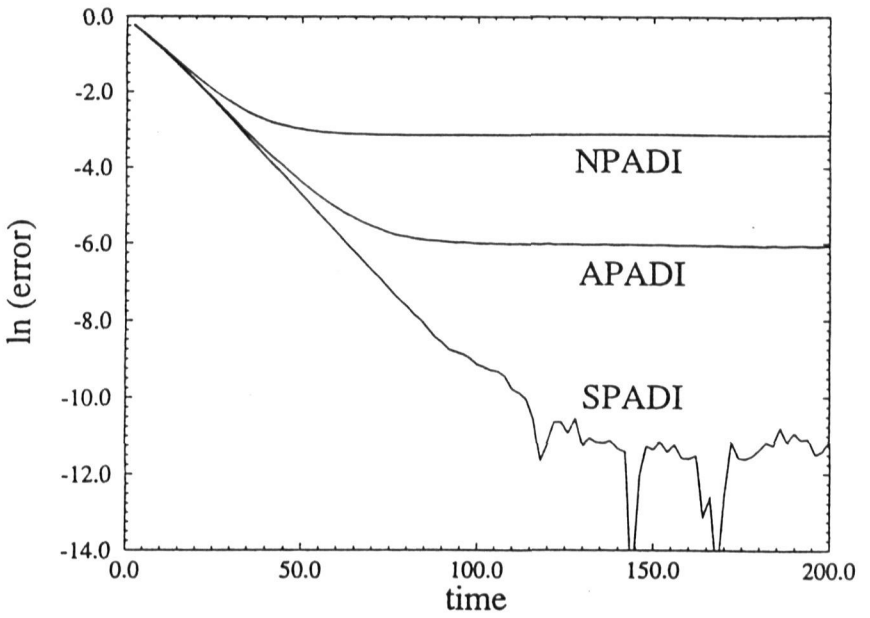

Figure 1. Fractional error in the ground state energy, found using first-order operator separation for an exactly separable problem.

A nonseparable example, illustrated below, is based on the total potential illustrated in figure 2 (piecewise constant: 0.0 eV in first and third quadrants, 0.2 eV in the remaining two, with hard walls around a square of side 400Å).

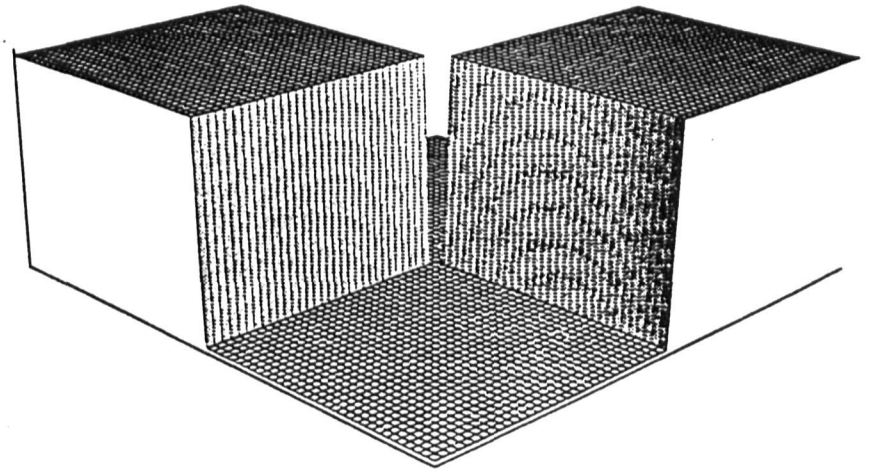

Figure 2. A nonseparable potential, with the x axis along the right-hand edge, and the y axis along the left-hand edge.

After relaxing toward a solution, V^x had the form shown in Fig. 3. Note that V^x is different for each energy level. The special case in which it is the same for every level is the usual case of a separable potential.

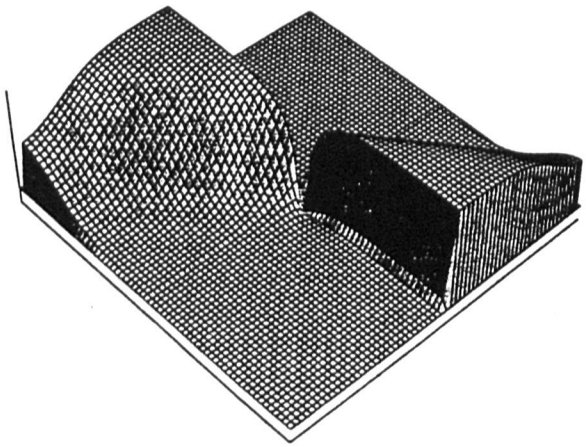

Figure 3. V^x for ground state of V in figure 2 (different scale, perspective; x-axis still to right)

The graph corresponding to Fig. 1, for the nonseparable potential, is Fig. 4. This calculation was done using a second-order ADI.

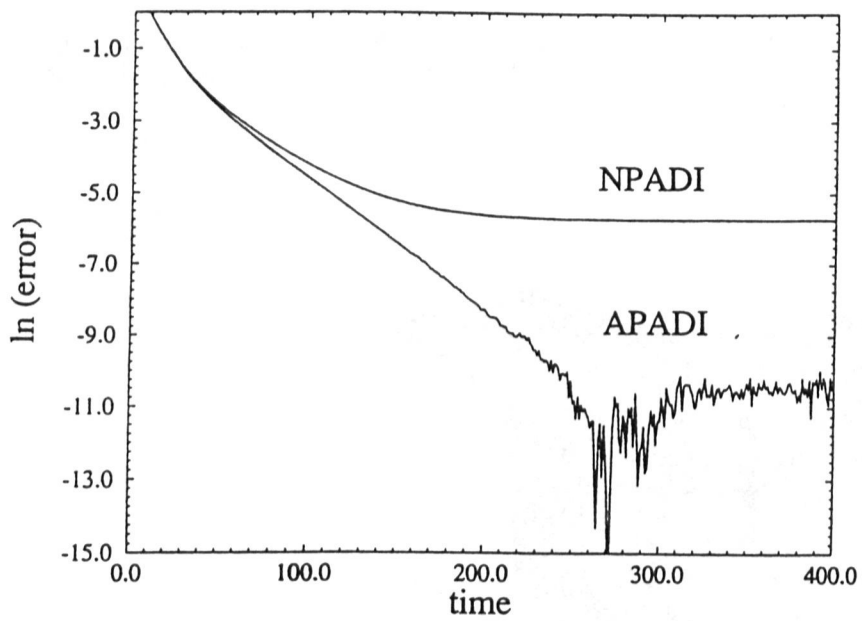

Figure 4. Fractional error for nonseparable potential.

References

[1] See, for example, W. H. Press, S. A. Teukolsky, W. T. Vetterling and B. P. Flannery, *Numerical Recipes in FORTRAN*, Cambridge Univ. Pr., 1986, 1992.

[2] S. Doss and K. Miller, "Dynamic ADI Methods for Elliptic Equations," SIAM J. Numer. Anal., Vol. 16, No. 5, pp. 837-856, October 1979.