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Efficient Finite Difference Solutions to the Time-Dependent Schrödinger Equation

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The matrix elements of the exponential of a finite difference realization of the one-dimensional Laplacian are found exactly. This matrix is used to formulate an efficient algorithm for the numerical solution to the time-dependent quantum mechanical scattering of a single particle from a time-independent potential in one-space and one-time dimension. The method generalizes to higher spatial dimensions, as well as to multiparticle problems. © 1997 Academic Press

1. INTRODUCTION

The problem of time-dependent quantum mechanical scattering of a spinless particle of mass m from a time-independent potential V in one-space and one-time dimension has a long and remarkable history. It is impossible to do justice to the many workers who have contributed to this topic in the opening paragraph of a short letter. However, it is well known that some of the most accurate and stable numerical techniques that provide time-dependent solutions to the scattering problem are based on unitary algorithms that often carry a large computational overhead. For example, Cayley's fractional form of the evolution operator $e^{-(i/\hbar)Ht}$ poses efficiency problems because of the inverse operator that appears in the approximation $e^{-(i/\hbar)Ht} = (1 - (i/2\hbar)\ Ht)(1 + (i/2\hbar)\ Ht)^{-1} + \cdots$ [1]. Fourier transform methods in which the kinetic energy operator is diagonal [2] depend on nonlocal transforms that are computationally expensive to perform. Alternating direction implicit techniques are often formulated in terms of tridiagonal systems that must be solved for each new time step [3]. Several other propagation schemes that are often employed, including the nonunitary Chebyshev expansion scheme are reviewed in [4]. Each, of course, has its advantages and disadvantages depending in large measure on the particular initial value problem under study.

Other more efficient unitary algorithms have been applied that are explicit and local [5, 6], but do not always achieve the same accuracy as the previous approaches. The algorithm that we shall discuss in this paper is also both explicit and local. Its novel features include the exact evaluation of a major contribution to an approximation to the evolution operator (Eq. (16)) and a first-order approximation to the exponential of the commutator of the kinetic energy operator with the potential energy operator. The algorithm based on these results yields efficient approximate finite difference solutions to the Schrödinger equation that are accurate to at least $O([\hbar\delta t/ma^2]^3)$, where δt is the time step and a is the uniform lattice spacing. This algorithm will provide efficient approximate solutions of increased accuracy for some initial value problems.

II. METHOD

The initial value problem is governed by the Schrödinger equation

$$-\frac{\hbar}{i}\frac{\partial}{\partial t}\Psi(x,t) = \frac{-\hbar^2}{2m}\nabla^2\Psi(x,t) + V\Psi(x,t) \qquad (1)$$

or

$$\partial_t\Psi = \left[\frac{i\hbar}{2m}\nabla^2 - \frac{iV}{\hbar}\right]\Psi, \qquad (2)$$

subject to prescribed initial data. We consider only time-independent potentials V so that $[\partial_t, V] = 0$ and

$$\Psi(x, t+\delta t) = e^{\delta t\partial_t}\Psi(x,t) = e^{(i\hbar\delta t/2m)\nabla^2 - iV\delta t/\hbar}\Psi(x,t). \qquad (3)$$

We may expand the evolution operator as

$$e^{(i\hbar\delta t/2m)\nabla^2 - iV\delta t/\hbar} = \cdots e^{A_3\delta t^3}\, e^{A_2\delta t^2}\, e^{-iV/\hbar}\, e^{(i\hbar/2m)\nabla^2}, \qquad (4)$$

where the A_2, A_3, ... are anti-Hermitian operators. For example, A_2 may be calculated by differentiating Eq. (4) twice with respect to δt and then setting $\delta t = 0$. This yields

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$$A_2 = \frac{1}{4m}[\nabla^2, V] = \frac{1}{4m}(V'' + 2V'\partial_x). \tag{5}$$

Consider now the scattering problem formulated on a discrete spatial lattice with a uniform lattice spacing a. Let integers $n, n', \ldots$ denote lattice site indices ($-\infty < n, n' \ldots < \infty$). Ψ now carries an implicit lattice site index, and we understand that $\Psi(x,t) \leftrightarrow \Psi_n(t)$, where $x = na$. We employ a standard finite difference realization of the Laplacian $\nabla^2 = a^{-2}T + O(a^2)$ in one dimension in which the matrix elements of T are given by

$$T_{nn'} = \delta_{nn'+1} - 2\delta_{nn'} + \delta_{nn'-1}. \tag{6}$$

Equation (3) then gives

$$\Psi(t + \delta t) = e^{\delta t \partial_t}\Psi(t) = e^{(i\lambda/2)T - i\lambda U}\Psi(t), \tag{7}$$

where we have put

$$\lambda = \hbar\delta t/ma^2 \tag{8}$$

and

$$U = (ma^2/\hbar^2)V. \tag{9}$$

We again expand the evolution operator as

$$e^{(i\lambda/2)T - i\lambda U} = \cdots e^{\lambda^3 B_3} e^{\lambda^2 B_2} e^{-i\lambda U} e^{(i\lambda/2)T}, \tag{10}$$

where the anti-Hermitian operators $B_2, B_3, \ldots$ may be determined as accuracy dictates. B_2 is calculated below. It is important to note that, to each order, the decomposition of the evolution operator is in terms of unitary operators, so that the norm of Ψ is preserved as the dynamics unfolds. A numerical algorithm based on this expansion will be unconditionally stable.

$e^{(i\lambda/2)T}$ may be calculated exactly. To this end we define an n'-parameterized family of special functions $f_n^{(n')}$ by

$$\frac{\partial}{\partial\lambda} f^{(n')} = \frac{i}{2} T f^{(n')}, \tag{11}$$

i.e.,

$$\frac{\partial}{\partial\lambda} f_n^{(n')} = \frac{i}{2}(f_{n+1}^{(n')} - 2f_n^{(n')} + f_{n-1}^{(n')}), \tag{12}$$

subject to the initial conditions $f_n^{(n')}(0) = \delta_{nn'}$. The solution to Eq. (11) is

$$f^{(n')}(\lambda) = e^{(i\lambda/2)T} f^{(n')}(0), \tag{13}$$

while Eq. (12) may be written as

$$2\frac{\partial}{\partial\lambda} e^{i\lambda} f_n^{(n')} = i[e^{i\lambda} f_{n-1}^{(n')} + e^{i\lambda} f_{n+1}^{(n')}]. \tag{14}$$

Using the recursion relations $2Z_\nu' = Z_{\nu-1} - Z_{\nu+1}$ of the Bessel functions [7, 8], one readily finds that the solution to Eq. (12) subject to the given initial conditions is

$$f_n^{(n')}(\lambda) = i^{n-n'} e^{-i\lambda} J_{n-n'}(\lambda). \tag{15}$$

To obtain $e^{(i\lambda/2)T}$ we observe that the nth component of Eq. (13) is $f_n^{(n')}(\lambda) = i^{n-n'}e^{-i\lambda}J_{n-n'}(\lambda) = \Sigma_{n''}[e^{(i\lambda/2)T}]_{nn''} f_{n''}^{(n')}(0) = \Sigma_{n''}[e^{(i\lambda/2)T}]_{nn''}\delta_{n''n'} = [e^{(i\lambda/2)T}]_{nn'}$, which we record as

$$[e^{(i\lambda/2)T}]_{nn'} = i^{n-n'}e^{-i\lambda}J_{n-n'}(\lambda). \tag{16}$$

Since U is diagonal we find that

$$[e^{(i\lambda/2)T - i\lambda U}]_{nn'} = [\cdots e^{-i\lambda U}e^{(i\lambda/2)T}]_{nn'} \approx i^{n-n'}e^{-i\lambda(1+U_n)}J_{n-n'}(\lambda), \tag{17}$$

so that to $O([\hbar\delta t/ma^2]^2)$,

$$\begin{aligned}
&\Psi_n(t + \delta t)\\
&= e^{-i\lambda(1+U_n)} \sum_{n'=-\infty}^{\infty} i^{n-n'} J_{n-n'}(\lambda)\Psi_{n'}(t)\\
&= e^{-i\lambda(1+U_n)} \sum_{n'=-\infty}^{\infty} i^{n'} J_{n'}(\lambda)\Psi_{n-n'}(t)\\
&= e^{-i\lambda(1+U_n)}\left[J_0(\lambda)\Psi_n(t) + \sum_{n'=1}^{\infty} i^{n'}J_{n'}(\lambda)[\Psi_{n-n'}(t) + \Psi_{n+n'}(t)]\right].
\end{aligned} \tag{18}$$

The $J_n(\lambda)$ are calculated only once at the beginning of the procedure. If one examines the asymptotic expansion of J_n then one sees that it decreases exponentially [7, 8] for large $|n/\lambda|$. Only a few need be included in a numerical approximation.

B_2 may be calculated by differentiating Eq. (10) twice with respect to λ and then setting $\lambda = 0$. This yields

$$B_2 = \tfrac{1}{4}[T, U], \tag{19}$$

which is a real antisymmetric matrix and, as stated above, is the generator of a unitary transformation. The matrix elements of B_2 are easily found to be

$$B_{2nn'} = \tfrac{1}{4}(U_{n+1} - U_n)(\delta_{nn'-1} - \delta_{nn'+1}). \tag{20}$$

We shall represent B_2 as the sum $B_2 = B_2^a + B_2^b$ of two (noncommuting) block-diagonal antisymmetric matrices B_2^a and B_2^b. We shall choose B_2^a and B_2^b so that each can individually be exponentiated to a finite rotation matrix that possesses a concise closed form. Let us consider the evalution of the unitary approximation $e^{\lambda^2 B_2} = [1 + O([\hbar\delta t/ma^2]^4)]\, e^{\lambda^2 B_2^b} e^{\lambda^2 B_2^a}$ under these conditions.

We express B_2^a as a direct sum,

$$B_2^a = \bigoplus_n'' S_n, \tag{21}$$

where $\oplus_n''$ denotes a sum over every other lattice site (so that n has definite parity),

$$S_n = \frac{1}{4}(U_{n+1} - U_n)\sigma \tag{22}$$

and

$$\sigma = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \tag{23}$$

Also

$$B_2^b = XLAT \circ \left[\bigoplus_{\bar{n}}'' S_{\bar{n}} \right]. \tag{24}$$

Here $\bar{n}$ in Eq. (24) has the opposite parity to n in Eq. (21). The translation operator $XLAT$ shifts the elements of B_2^b relative to B_2^a down one row and right one column. Each of the two block-diagonal antisymmetric matrices B_2^a and B_2^b generates a family of rotations connecting disjoint ordered pairs of adjacent nodes (Ψ_n, Ψ_{n+1}), where each Ψ_n is included only once for B_2^a and only once for B_2^b. At a lattice site n, Ψ_n is paired with Ψ_{n-1} for one of these rotations, and with Ψ_{n+1} for the other.

To clarify this construction let us consider a concrete example. We truncate the lattice to $2N + 1$ sites, $N > 0$, so that $-N \le n, n' \le N$. Then

$$B_2^a = S_{-N} \oplus S_{-N+2} \oplus \cdots \oplus S_{N-2} \oplus 0_{1\times 1} \tag{25}$$

and

$$B_2^b = 0_{1\times 1} \oplus S_{-N+1} \oplus S_{-N+3} \oplus \cdots \oplus S_{N-1}. \tag{26}$$

The leading 1×1 block of zero, $0_{1\times 1}$, in the last equation shifts the elements of B_2^b relative to B_2^a down one row and right one column, while the terminal $0_{1\times 1}$ block in B_2^a makes it the same size as B_2^b.

Let $\theta_n = (\lambda^2/4)(U_{n+1} - U_n)$. In order to describe the actions of the two rotations B_2^a and B_2^b let us assume that n and N have the same parity. If $n \neq N$ then under the action of B_2^a the ordered pair (Ψ_n, Ψ_{n+1}) transforms into $\Psi_n \to \Psi_n \cos(\theta_n) + \Psi_{n+1} \sin(\theta_n)$ and $\Psi_{n+1} \to -\Psi_n \sin(\theta_n) + \Psi_{n+1} \cos(\theta_n)$; if $n = N$ then Ψ_n is invariant under this rotation (Ψ_n maps to Ψ_n). This is followed by $e^{\lambda^2 B_2^b}$ which rotates the ordered pair (Ψ_{n-1}, Ψ_n) into $\Psi_{n-1} \to \Psi_{n-1} \cos(\theta_{n-1}) + \Psi_n \sin(\theta_{n-1})$ and $\Psi_n \to -\Psi_{n-1} \sin(\theta_{n-1}) + \Psi_n \cos(\theta_{n-1})$, unless $n = -N$. If $n = -N$ then Ψ_n is invariant under the action of B_2^b.

III. CONCLUSION

In order to generalize this method to two spatial dimensions we replace Ψ_n with $\Psi_{n_x n_y}$ and the kinetic energy operator $T_{nn'}$ with $T_{n_x n_x'}\delta_{n_y n_y'} + T_{n_y n_y'}\delta_{n_x n_x'}$, if the lattice spacing is a for both axes. Otherwise $\lambda T_{nn'} \to \lambda_x T_{n_x n_x'}\delta_{n_y n_y'} + \lambda_y T_{n_y n_y'}\delta_{n_x n_x'}$, where $\lambda_x = (\hbar/ma_x^2)\,\delta t$ and $\lambda_y = (\hbar/ma_y^2)\,\delta t$. The potential energy operator is still diagonal, $\lambda U_n \to (\delta t/\hbar)V_{n_x n_y}$. The evolution operator $e^{-(i/\hbar)Ht}$ applied to the state vector at time t yields

$$\Psi_{n_x n_y}(t + \delta t) = e^{-i(\lambda_x + \lambda_y + \delta t/\hbar V_{n_x n_y})} \sum_{n_x'=-\infty}^{\infty} \sum_{n_y'=-\infty}^{\infty} i^{n_x - n_x'} i^{n_y - n_y'} J_{n_x - n_x'}(\lambda_x) J_{n_y - n_y'}(\lambda_y) \Psi_{n_x' n_y'}(t), \tag{27}$$

to $O([\hbar\delta t/ma^2]^2)$. Increased accuracy may be obtained by including the B_2 dependent terms. The $J_n(\lambda)$ are calculated only once. They fall off exponentially for large $|n/\lambda|$. In practice only a few of the $J_n(\lambda)$ need be retained. While λ is arbitrary, its value should be tuned to an optimal value once the lattice spacing and potential energy are given. For example, if one picks λ to be the first zero of J_0 then one should expect to have to retain more terms in the sum of Bessel functions to achieve a desired accuracy.

The two particle problem in one spatial dimension follows directly from the single particle theory in two spatial dimensions when the two particles are distinguishable. Let the masses of the two particles be m_1 and m_2. We identify λ_x with $(\hbar/m_1 a^2)\,\delta t$ and λ_y with $(\hbar/m_2 a^2)\,\delta t$, and proceed in the obvious manner. Many higher order (in particle number and/or spatial dimension) problems may be handled by a straightforward extension of these ideas.

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