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A Comparison of Methods for Determining the Time Step When Propagating with the Lanczos Algorithm

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Abstract: To use the short iterative Lanczos algorithm to solve the time-dependent Schroedinger equation, one must choose, for a given Lanczos space size, a time step. We compare the derivation of the well-known Lubich and Hochbruck time step from SIAM J. Numer. Anal. 34 (1997) 1911 with the a priori time step we proposed in Mohankumar and Carrington (MC) Comput. Phys. Commun., 181 (2010) 1859 and demonstrate that the MC time step is somewhat larger, i.e., that the MC error bound is tighter. In addition, we use the MC approach to derive an error bound and time step for imaginary time propagation. The error bound we derive is much tighter than the error bound of Stewart and Leyk.

Keywords: short iterative Lanczos algorithm; propagation; Chebyshev error bounds

1. Introduction

The short iterative Lanczos (SIL) algorithm [1] for solving the time-dependent Schroedinger equation (TDSE) (in atomic units),

$$i \frac{\partial}{\partial t} \psi(x, t) = \hat{H} \psi(x, t), \quad (1)$$

is widely used in chemical physics and other fields. To solve the TDSE, the first step is to represent \hat{H} and $\psi(x, t)$ in a (here orthonormal) basis, to obtain,

$$i \frac{\partial \mathbf{a}(t)}{\partial t} = \mathbf{H} \mathbf{a}(t), \quad (2)$$

where

$$\psi(x, t) = \sum_k a_k(t) \phi_k(x), \quad (3)$$

and

$$H_{k',k} = \langle \phi_{k'} | H | \phi_k \rangle. \quad (4)$$

solving the TDSE enables one to compute photodissociation cross section, rate constants, etc. [2–7]. To use SIL, Equation (2) is solved by writing $\mathbf{a}(t) = \mathbf{Q}_m \mathbf{c}(t)$, and computing

$$\mathbf{c}(t) = \mathbf{Q}_m^T \mathbf{a}(t) \approx e^{-it\mathbf{T}_m} \mathbf{c}(0), \quad (5)$$

where \mathbf{Q}_m is the matrix of m Lanczos vectors,

$$\mathbf{H}\mathbf{Q}_m = \mathbf{Q}_{m+1}\hat{\mathbf{T}}_m, \tag{6}$$

and $\hat{\mathbf{T}}_m$ is a tridiagonal matrix,

$$\hat{\mathbf{T}}_m = \begin{bmatrix} \alpha_1 & \beta_1 & 0 & \cdots & 0 \\ \beta_1 & \alpha_2 & \beta_2 & \cdots & 0 \\ 0 & \beta_2 & \alpha_3 & \beta_3 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \cdots & \beta_{m-2} & \alpha_{m-1} & \beta_{m-1} \\ 0 & \cdots & 0 & \beta_{m-1} & \alpha_m \\ 0 & \cdots & 0 & 0 & \beta_m \end{bmatrix}. \tag{7}$$

Note that

$$\mathbf{T}_m = \mathbf{Q}_m^T \mathbf{H} \mathbf{Q}_m. \tag{8}$$

The notation used here is the same as the notation of [8]. m is small enough that loss of orthogonality of the Lanczos vectors is unimportant. In this paper, we shall assume that $\mathbf{a}(t = 0)$ is the Lanczos starting vector. In that case

$$\mathbf{c}(0) = \mathbf{c}_0 = \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}. \tag{9}$$

To use the SIL algorithm, one chooses a value of m , propagates from $t = 0$ to $t = \Delta t$, and then uses $\mathbf{a}(\Delta t)$ as the starting vector and propagates again from $t = \Delta t$ to $t = 2\Delta t$, etc. For a fixed m , small enough that loss of orthogonality is not a problem, one must choose Δt . It is advantageous to make Δt as large as possible, but Δt must be chosen so that the size of the error at each step is acceptably small. Mathematicians tend to be familiar with the approach of Lubich (L) and Hochbruck [9–11] for choosing Δt .

In 2010, we (Mohankumar and Carrington—MC) derived a slightly different equation for choosing Δt [8]. In this paper, we compare the derivations of the Lubich and MC equations and show that Δt^{MC} is somewhat larger than Δt^L and therefore that using Δt^{MC} reduces the cost of propagating. In addition, we derive and test a new equation for Δt for propagating in imaginary time.

2. Comparing the Derivations

2.1. Common Starting Point

Although the L and MC equations for Δt are very similar, their derivations are different. Both derivations begin with a link between an error bound for a Lanczos approximation to a function of a matrix applied to a vector and an error for an approximation of the same function by a polynomial of a certain degree. In [8], we began with a result of Stewart and Leyk [12]. It is very similar to Theorem 2.9 of [9]. According to Theorem 2.9, for any complex-valued function f defined on an interval $[a, b]$ that contains the eigenvalues of the Hermitian matrix \mathbf{A} , the error of the Lanczos approximation to $f(\mathbf{A})\mathbf{v}$ is bounded by

$$\|\mathbf{Q}_m \mathbf{f}(\mathbf{T}_m) \mathbf{e}_1 - f(\mathbf{A})\mathbf{v}\| \leq 2 \inf_{p_{m-1}} \max_{x \in [a,b]} |p_{m-1}(z) - f(z)|. \tag{10}$$

Here, \mathbf{v} is a unit vector and the infimum is taken over all polynomials of degree at most $(m - 1)$. The corresponding lemma of Stewart and Leyk (Lemma 2, [12]) is similar, but derived differently, using the min-max theorem for symmetric matrices. It is

$$\|e^{-\mathbf{A}\mathbf{v}} - \mathbf{Q}_m \mathbf{e}^{-\mathbf{T}_m \mathbf{Q}_m^T \mathbf{v}}\|_2 \leq 2\|\mathbf{v}\|_2 \|\mathbf{r}\|, \tag{11}$$

where

$$\|\mathbf{r}\| = \min \max \left\{ |e^{-\lambda} - p_{m-1}(\lambda)|; \lambda \in [\lambda_{min}, \lambda_{max}] \right\}, \tag{12}$$

and λ_{min} and λ_{max} are the minimum and maximum eigenvalues of \mathbf{A} .

2.2. Lubich Derivation

Lubich combines his Theorem 2.9 with a bound on $|p_{m-1}(x) - e^{i\omega x}|$ (his Theorem 2.2) to derive a bound on the error. He finds that for any Hermitian matrix, \mathbf{H} , all of whose eigenvalues are in the interval $[a, b]$, the error of the Lanczos method is bounded by

$$\epsilon_b^{HL} = \|\mathbf{Q}_m e^{-i\Delta t \mathbf{T}_m \mathbf{e}_1} - e^{-i\Delta t \mathbf{H} \mathbf{v}}\| \leq 8 \left(e^{1 - (\omega/2m)^2} \frac{|\omega|}{2m} \right)^m; m \geq |\omega|; \omega = \Delta t(b - a)/2, \tag{13}$$

where \mathbf{v} be a vector of unit Euclidean norm. Δt^{HL} is derived by setting $y = |\omega|/2m = (b - a) \Delta t/4m$, replacing the above inequality by an equality, and solving iteratively the following equation

$$\epsilon_b^{HL} = 8 \left(e^{1 - y^2} y \right)^m = \left\{ 8 e^{-my^2} \right\} \alpha^m, \tag{14}$$

where $\alpha = ey$.

2.3. Mohankumar-Carrington Derivation

MC replace $p_{m-1}(x)$ in Equation (11) with a Chebyshev [13] approximation for $e^{-i\omega x}$ which is,

$$J_0(\omega)T_0(x) + \sum_{n=1}^{m-1} (-i)^n 2J_n(\omega)T_n(x).$$

In Equation (11), it is the difference of the exact function $e^{-i\omega x}$ and the polynomial (here a Chebyshev polynomial) of degree $(m - 1)$ that appears. We therefore need an estimate of the remainder $R_m = \sum_{n=m}^{\infty} (-i)^n 2J_n(\omega)T_n(x)$. Since the modulus of $T_n(x)$ cannot exceed unity, we get

$$|R_m| < \sum_{n=m}^{\infty} |2J_n(\omega)|. \tag{15}$$

In the Appendix A, we show that

$$J_n(x) < \frac{1}{\sqrt{2\pi n}} (ex/2n)^n. \tag{16}$$

It is straightforward to obtain a closed-form expression that bounds the right hand side (RHS) of Equation (15), by using Equation (16) and summing a geometric series. This is explained in [8]. We obtain

$$\epsilon_b^{MC} = \left\{ \sqrt{\frac{8}{\pi m}} \frac{1}{(1 - \alpha)} \right\} \alpha^m. \tag{17}$$

In both Equations (17) and (14), the dominant term is α^m . In typical calculations, Δt is small enough that $1 - \alpha \sim 1$ and $e^{-my^2} \sim 1$ and in this case the time step Δt^{MC} is larger than Δt^L by a factor of $(8\pi m)^{1/m}$. Δt^{MC} is larger than Δt^L whenever $\alpha < 0.8$.

3. Test Calculations for Real-Time Propagation

To test the ideas, we propagated a Gaussian wave packet in a 1D harmonic potential. The Hamiltonian (atomic units are used) is

$$H = \frac{p^2}{2m_0} + \frac{1}{2}m_0\omega^2x^2, \tag{18}$$

where $m_0 = 1$ and $\omega = 2.7338 \times 10^{-4}$, corresponding to a wavenumber of 60 cm^{-1} . The starting wave packet is displaced from equilibrium by $x_0 = 56$:

$$\psi(x, 0) = \frac{\alpha_0^{1/2}}{\pi^{1/4}} e^{-\alpha_0^2(x-x_0)^2/2} \tag{19}$$

$$\alpha_0 = [m_0k/\hbar^2]^{1/4}; \omega = (k/m_0)^{1/2}. \tag{20}$$

The exact solution is known [14],

$$\|\psi(x, t)\|^2 = \frac{\alpha_0}{\sqrt{\pi}} e^{-\alpha_0^2[x-x_0 \cos(\omega t)]^2}. \tag{21}$$

The Hamiltonian matrix was constructed using the sinc discrete variable representation (DVR) of [15]. The size of the matrix is 80. We set $m = 22$. The DVR points are between -550 and $+550$ bohr. The spectral range is $(b - a) = 0.0309$ hartree.

Absolute values of relative errors in the propagated wave packet are shown in Table 1. The errors are at the values of x in the first column. There is one pair of columns for each ϵ . The first member of a pair contains errors computed with the MC time step; the second member of a pair contains errors computed with the L time step. The MC time step is somewhat larger, but the MC and L errors are comparable. Both errors are small. The total time for which the wave packet is propagated is approximately the same for an MC and L column with the same ϵ . Table 2 gives Δt^{MC} , Δt^L , and the percentage increase for several ϵ values. When $\epsilon \leq 10^{-10}$, Δt^{MC} is about 10% larger.

Table 1. Results of the comparison of the time-step criteria.

Time-Step	689.11	661.6	566.49	526.1	463.57	421.5	378.35	339.3
Iterations	200	208	200	215	200	220	200	220
ϵ/x	10^{-4}	10^{-4}	10^{-6}	10^{-6}	10^{-8}	10^{-8}	10^{-10}	10^{-10}
12	1.298×10^{-6}	1.081×10^{-6}	4.925×10^{-9}	2.029×10^{-9}	2.319×10^{-10}	3.604×10^{-11}	3.287×10^{-12}	7.618×10^{-13}
23	1.149×10^{-7}	4.520×10^{-7}	3.644×10^{-8}	6.550×10^{-14}	3.314×10^{-10}	2.538×10^{-11}	8.968×10^{-13}	1.617×10^{-12}
58	4.238×10^{-7}	3.929×10^{-7}	6.506×10^{-9}	1.114×10^{-9}	2.821×10^{-11}	5.802×10^{-12}	4.718×10^{-12}	1.077×10^{-12}
89	6.756×10^{-7}	1.854×10^{-7}	2.126×10^{-11}	1.396×10^{-10}	7.604×10^{-11}	2.442×10^{-12}	7.601×10^{-12}	1.121×10^{-12}
120	9.161×10^{-7}	3.006×10^{-7}	4.231×10^{-9}	8.909×10^{-10}	1.044×10^{-10}	1.852×10^{-11}	5.667×10^{-12}	1.712×10^{-12}
200	4.398×10^{-7}	2.536×10^{-7}	3.462×10^{-9}	3.918×10^{-10}	9.433×10^{-11}	1.276×10^{-11}	1.619×10^{-12}	1.741×10^{-12}
400	1.931×10^{-6}	5.332×10^{-7}	3.017×10^{-7}	3.502×10^{-8}	1.824×10^{-10}	2.030×10^{-11}	9.238×10^{-11}	1.605×10^{-13}

Table 2. Comparison of time-step sizes.

ϵ	Δt^{MC}	Δt^L	Percentage Increase
1×10^{-4}	6.891×10^2	6.616×10^2	4.15
1×10^{-6}	5.665×10^2	5.261×10^2	7.68
1×10^{-8}	4.632×10^2	4.215×10^2	9.97
1×10^{-10}	3.784×10^2	3.393×10^2	11.5
1×10^{-12}	3.083×10^2	2.739×10^2	12.6
1×10^{-14}	2.509×10^2	2.214×10^2	13.3

4. Imaginary Time Propagation

It is sometimes necessary to compute $\exp(-\mathbf{A})\mathbf{v}$, where \mathbf{A} is a real matrix. This is done, for example, to compute the ground state of a quantum system [16]. Using the Chebyshev approach, we can derive an error bound for the imaginary time propagation.

4.1. An Error Bound from a Geometric Series

It is straightforward to derive a Chebyshev expansion of $e^{-\omega x}$, where ω is real, $\omega > 0$, and x is between -1 and $+1$. The expansion coefficients are obtained from the integral [17]

$$\int_{-1}^1 \frac{e^{-\omega x} T_n(x) dx}{\sqrt{1-x^2}} = (-1)^n \pi I_n(\omega), \tag{22}$$

where $I_n(\omega)$ is a modified Bessel function of the first kind. The expansion is

$$e^{-\omega x} = \sum_{j=0}^{\infty} a_j(\omega) T_j(x), \tag{23}$$

where

$$a_0(\omega) = I_0(\omega); a_j = (-1)^j 2 I_j(\omega). \tag{24}$$

To use Equation (10) to bound $\|\mathbf{Q}_m e^{-\Delta t \mathbf{T}_m} \mathbf{e}_1, -e^{-\Delta t \mathbf{H}} \mathbf{v}\|$, we use a Chebyshev expansion of $e^{-\Delta t z}$, $\Delta t > 0; z \in [a, b]$. Both Δt and z are real. The expansion is obtained by mapping z onto x , using $z = (a+b)/2 + x(b-a)/2$. We find,

$$e^{-\Delta t z} = e^{-(\Delta t/2)(a+b)} \left\{ I_0(\omega) + 2 \sum_{j=1}^{\infty} (-1)^j I_j(\omega) T_j(x) \right\}; \omega = (\Delta t/2)(b-a). \tag{25}$$

If we truncate the series after $j = (m - 1)$, then the remainder is

$$R_m = 2 e^{-(\Delta t/2)(a+b)} \sum_{j=m}^{\infty} (-1)^j I_j(\omega) T_j(x). \tag{26}$$

Hence, the bound on R_m is

$$|R_m| \leq 2 e^{-(\Delta t/2)(a+b)} \sum_{j=m}^{\infty} |I_j(\omega)|. \tag{27}$$

If the argument ω of $I_n(\omega)$ is real, then (9.6.3, Abramowitz and Stegun, page 375 [18]),

$$I_j(\omega) = e^{-ij\pi/2} J_j(i\omega). \tag{28}$$

We now use the asymptotic expression for $|J_n(\omega)|$ (Abramowitz and Stegun, 9.3.1 [18]):

$$|I_n(\omega)| = |e^{-in\pi/2} J_n(i\omega)| = |J_n(i\omega)| \sim \frac{1}{\sqrt{2\pi n}} (e\omega/2n)^n. \tag{29}$$

When $\omega > 0$, the sum in Equation (27) is therefore bounded by a geometric series (as is true for the real-time case)

$$\left| \sum_{j=m}^{\infty} I_j(\omega) \right| < \frac{1}{\sqrt{2\pi m}} \frac{\left[\frac{e\omega}{2m} \right]^m}{\left(1 - \frac{e\omega}{2m} \right)}, \tag{30}$$

and $|R_m|$ itself is bounded by

$$|R_m| \leq 2 e^{-(\Delta t/2)(a+b)} \frac{1}{\sqrt{2\pi m}} \frac{\left[\frac{e\omega}{2m}\right]^m}{\left(1 - \frac{e\omega}{2m}\right)}. \tag{31}$$

The geometric series converges only if $(e\omega/(2m)) = (e\Delta t/(4m))(b - a) < 1$. Including the factor of two in Equation (10), we find that the error bound is

$$\epsilon = 4 e^{-(\Delta t/2)(a+b)} \frac{1}{\sqrt{2\pi m}} \frac{\left[\frac{e\omega}{2m}\right]^m}{\left(1 - \frac{e\omega}{2m}\right)}. \tag{32}$$

This is much simpler than the bound given by Stewart and Leyk [12].

4.2. An Error Bound from the First Term in Equation (27)

According to Equation (29), for a fixed z , $J_m(z) \sim 1/m^{m+1/2}$. Hence, the first term in the series in Equation (27) is the largest. If it is significantly larger, then the first term, by itself, can be used to bound the error. If we use Equation (29) and keep only the first term, we find the error bound,

$$E1 = \epsilon = 4 e^{-(s/2)(a+b)} I_m(\omega). \tag{33}$$

Note that the error bound of Equation (32) is only valid if $(e\Delta t/(4m))(b - a) < 1$, but that the error bound of Equation (33) has no such constraint.

4.3. Test Calculations

For the case $e^{-\mathbf{A}}$, where \mathbf{A} is real and symmetric (which corresponds to imaginary time propagation), we tested Equations (32) and (33) using the $n \times n$ diagonal matrix $\mathbf{A} = \mathbf{A}_2$, used to test the error bound of SL [12]. Its elements are $d(1) = 1$, $d(n) = 1 + c$, $c > 0$, and $d(j) = 1 + cx_j$, $j = 2, 3, \dots, (n - 1)$, $0 < x_j < 1$, where x_j is a uniformly distributed random number between 0 and 1. The minimum and maximum diagonal entries are $d(1)$ and $d(n)$, which are also the minimum and maximum eigenvalues. We calculate the Lanczos approximation for $e^{-\mathbf{A}_2 \mathbf{v}}$, where \mathbf{v} is a column vector of unit norm. It is $\mathbf{Q} e^{-\Lambda} \mathbf{Q}^T \mathbf{v}$, where $\mathbf{Q} = \mathbf{Q}_m \mathbf{U}$ and $\mathbf{U}^T \mathbf{T}_m \mathbf{U} = \Lambda$ (notation of Equation (6)). In Table 3, we give exact values of $Err = |e^{-\mathbf{A}_2 \mathbf{v}} - \mathbf{Q} e^{-\Lambda} \mathbf{Q}^T \mathbf{v}|$ for various values of n, m and c , and also the errors calculated with Equation (30) and Equation (33). Note that here $\Delta t = 1$. When c is large, the condition $(e\Delta t/4m)(b - a) < 1$ is not satisfied and we cannot sum the geometric series that leads to the error $E2$. The corresponding entries in the table are missing. According to Table 3, the $E2$ bound is conservative and the $E1$ bound given by Equation (33) is quite good. Both the error bounds we derive are much tighter than the error bound of Stewart and Leyk (their Equation (23)).

Table 3. Comparison of the error bounds of Equations (33) and (32) for imaginary time propagation. n is the size of the matrix; m is the size of the tridiagonal matrix; c is a parameter in A_2 ; and $\text{Err} = |e^{-A_2 v} - Qe^{-\Lambda}Q^T v|$.

n	m	c	Err	Equation (33)	Equation (32)	SL Error
100	12	8	9.848×10^{-8}	3.125×10^{-7}	4.243×10^{-7}	$\times 10^{-3}$
100	22	8	6.149×10^{-16}	1.196×10^{-16}	1.341×10^{-16}	3.545×10^{-3}
100	22	18	1.484×10^{-11}	9.009×10^{-11}	8.576×10^{-11}	1.437×10^{-6}
200	12	6	7.919×10^{-9}	2.357×10^{-8}	3.027×10^{-8}	1.848×10^{-2}
200	20	8	4.160×10^{-15}	1.404×10^{-14}	1.602×10^{-14}	3.545×10^{-3}
200	20	40	2.594×10^{-6}	9.672×10^{-6}	---	2.476×10^{-2}
400	12	5	1.213×10^{-9}	4.136×10^{-9}	5.155×10^{-9}	4.219×10^{-2}
400	20	5	2.685×10^{-15}	4.638×10^{-18}	5.209×10^{-18}	4.219×10^{-2}
1200	100	20	1.751×10^{-14}	7.231×10^{-93}	6.541×10^{-93}	1.766×10^{-7}
1200	100	40	2.842×10^{-14}	8.706×10^{-67}	4.467×10^{-67}	1.191×10^{-14}
4000	12	15	1.224×10^{-5}	3.731×10^{-5}	8.790×10^{-5}	2.094×10^{-2}
4000	32	15	4.078×10^{-15}	1.105×10^{-20}	1.064×10^{-20}	1.096×10^{-5}

5. Conclusions

In this paper, we review and contrast two approaches [8,9] for bounding the error of a Lanczos approximation to $\exp(-it\mathbf{H})\mathbf{v}$, where \mathbf{H} is a real matrix, t is a real constant, and \mathbf{v} is a real vector. In physics applications, t is the time. Once an error bound has been found, it is straightforward to derive an equation for the best time step to use. The time step obtained from the MC approach [8] is slightly larger. This means that the cost of the the propagation with the MC time step is slightly less. In addition, we used the MC approach to derive an error bound (and time step) for the case when t in $\exp(-it\mathbf{H})$ is imaginary. The derivation is much simpler than the previous derivation in [12] and the error bound is much tighter.

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Appendix A

We use Equation (16)

$$J_n(x) < \frac{1}{\sqrt{2\pi n}} \left(\frac{xe}{2n}\right)^n; \quad n = 1, 2, \dots$$

to derive Equation (17), the error bound for real-time propagation. Here, n is a positive integer and x is real positive value. This relation has not previously been proved. The standard result for the bound on the Bessel function is (Equations 9.1.62 in Ref. [18])

$$|J_\nu(z)| \leq \frac{|\frac{z}{2}|^\nu e^{|\text{Im}(z)|}}{\Gamma(\nu + 1)}; \quad \nu \geq (-1/2), \tag{A1}$$

where z is complex. When ν is a positive integer and $z = x$ is real, Equation (A1) reduces to

$$|J_n(x)| \leq \frac{|\frac{x}{2}|^n}{n!}. \tag{A2}$$

An exact expression for $n!$ is given by [19]

$$n! = \sqrt{2\pi} n^{n+(1/2)} e^{-n} e^{r_n}; \quad n = 1, 2, \dots, \quad (\text{A3})$$

for some r_n in the range

$$\frac{1}{12p+1} < r_p < \frac{1}{12p}. \quad (\text{A4})$$

Since $e^{r_p} > 1$, the two equations above imply

$$n! > \sqrt{2\pi} n^{n+(1/2)} e^{-n}; \quad n = 1, 2, \dots \quad (\text{A5})$$

In view of Equations (A1) and (A5), we get for $x > 0$

$$\begin{aligned} J_n(x) &\leq \frac{1}{n!} (x/2)^n < \frac{(x/2)^n}{\sqrt{2\pi n} n^n e^{-n}} \\ &< \frac{1}{\sqrt{2\pi n}} \left(\frac{xe}{2n}\right)^n; \quad n = 1, 2, \dots \end{aligned}$$

Surprisingly, the RHS is exactly equal to the usual asymptotic relation for Bessel functions (Equations 9.3.1 in Ref. [18]).

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