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Chebyshev Approximation for Wave Packet Dynamics: better than expected

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Abstract

The aim of this work is to study the accuracy and stability of the Chebyshev approximation method as a time–discretization for wave packet dynamics. For this frequently used discretization we introduce estimates of the approximation and round–off error. These estimates mathematically confirm the stability of the Chebyshev approximation with respect to round–off errors, especially for very large stepsizes. But the results also disclose threads to the stability due to large spatial dimensions. All theoretical statements are illustrated by numerical simulations of the harmonic quantum oscillator.

Keywords: Round–off errors, Chebyshev approximation, Chebyshev polynomials, Faber polynomials, wave packet dynamics, fast Fourier transform.

AMS classification: 65L20, 81V55, 92C40

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1 Introduction

Computational simulations of molecular dynamics have to cope with a variety of elementary processes. To a certain degree, some of them can be modelled using classical mechanics. Others, like tunneling or zero-point energy effects in a molecule, require a quantum–mechanical description. In this case one seeks a solution of the time–dependent Schrödinger equation, i.e., a partial differential equation (PDE):

$$i\,\hbar\,\dot{\psi} \;=\; H_d\,\psi \tag{1}$$

where H_d denotes a selfadjoint Hamilton operator.

Unfortunately, these time–dependent quantum mechanical simulations cause even for small systems a huge numerical effort. Thus, one is interested in the use of efficient and numerically stable algorithms for both: the time– and the spatial discretization. In this paper we want to confine ourself on a rigorous investigation of one popular time–discretization under the assumption, that (1) is already spatially discretized by Fourier–(pseudo-)spectral or Fourier–collocation methods [1, 2, 3]. Thus, we suppose that (1) is a d-dimensional system of ordinary differential equations and H_d denotes the $d \times d$ matrix–representation of the Hamilton operator.

One method widely used for solving (1) is the Chebyshev approximation technique [4]. In this method the corresponding propagation operator $\exp(-itH_d)$ of (1) is expanded in a truncated series of Chebyshev polynomials. Analytically, a suitable increase of the order of the method, i.e., the number of expansion terms, allows us to meet any accuracy requirement, even for large timesteps. Interestingly, an increase of the stepsize in time reduces the computational work per unitstep. In consequence, the stepsizes (and, thus, expansion orders) typically used in real life applications are quite large.

Thus, the question arises whether increasing the order of the method yields unstabilities due to a simultaneously increasing round–off error. Mainly, this round–off error is produced by the large number of Fast–Fourier–Transforms used for the calculation of the Chebyshev polynomials. At worst, one could expect a tremendously growing round–off error for increasing orders of the Chebyshev method, an effect, which is observed for other expansion techniques (cf. Section IV). For this reason we present a rigorous estimation of the approximation error and the round–off-error. The results demonstrate that the round–off-error is increasing very mildly with the stepsize applied. There is no exploding amplification of the round–off error. In application to the Schrödinger equation, the Chebyshev–method is *better than expected* concerning the round–off error. The previous statement describes the *relative dependence* of the round–off error on the stepsize for *fixed* spatial grid dimension d. Unfortunately, the specific *magnitude* of the round–off error strongly depends on d, i.e., large grid dimensions can lead to severe restrictions on the achievable accuracy.

This paper is organized in the following way. Section II briefly describes the Chebyshev–approximation method. In Section III we present the estimates of approximation and round–off error and discuss the algorithmic consequences. For the sake of clarity the details of the calculation of the round–off error are referred to an appendix. Section IV illustrates the consequences of these results via some numerical simulations.

2 Chebyshev Expansion

The solution to the space–discretized Schrödinger equation (1) has the form

$$\Psi(\tau) \;=\; \exp\left(-i\, H_d\, t\right)\Psi_0. \tag{2}$$

Because of numerical instabilities of methods using truncated Taylor series to evaluate the matrix exponential function for large dimensions and large timesteps one is interested in efficient and numerically stable approximations of the propagator $\exp(-i\, H_d\, \tau)$ for a suitable time step τ. One of the most promising approaches is the expansion in Chebyshev polynomials [4]. This is due to the fact, that the evaluation of Chebyshev polynomials $T_k(x)$ can be done numerically stable for $|x| \leq 1$ via the recurrence relation:

$$T_{k+1}(x) = 2\, x\, T_k(x) - T_{k-1}(x); \qquad T_1(x) = x; \qquad T_0(x) = 1.$$

The matrix representation of the Hamiltonian operator H_d has a bounded spectrum. Thus, it is possible to transform the spectrum of the Hamiltonian into the *open* interval $]-1,1[$:

$$H = \frac{1}{r} H_d \qquad \text{so that} \qquad \sigma(H) \subset]-1,1[. \tag{3}$$

This transformation can be done by analyzing the spectral radius of H_d or, more simply, by calculating the energy range, which corresponds to the potential and the spatial discretization chosen [4]. For a problem with one degree of freedom, i.e., one space dimension before spatial discretization, the latter yields:

$$r = E_{\max} - E_{\min} = \frac{\pi^2 \hbar^2 d^2}{2\, m\, L^2} + V_{\max} - V_{\min},$$

where d and L denote the spatial grid dimension and the length of the spatial interval respectively. Note, that the notation used differs slightly from customary presentations of the method in order to support our further argumentation. However, we obtain:

$$\exp\left(-i\, H_d\, \tau\right) \Psi_0 = \exp\left(-i\, H\, r\, \tau\right) \Psi_0. \tag{4}$$

To avoid restrictions on the stepsize due to stability reasons one expands (4) in Chebyshev polynomials in the operator H instead of $Hr\tau$. Therefore we get:

$$\exp(-i\, H\, r\, \tau) \Psi_0 = \Big(\sum_{k=0}^{\infty} c_k(r\tau)\, T_k(H) \Big) \Psi_0. \tag{5}$$

Thus,

$$P_N(r\tau\, H) \Psi_0 = \Big(\sum_{k=0}^{N} c_k(r\tau)\, T_k(H) \Big) \Psi_0 \tag{6}$$

denotes the Chebyshev approximation of the order N. Analytically, the expansion coefficients c_k are determined via the orthogonality relation of the Chebyshev polynomials:

$$c_k(r\tau) = \frac{2}{(1 + \delta_{k0})} (-i)^k\, J_k(r\tau) \tag{7}$$

where J_n denotes the nth Bessel function. The reader should note that the expansion coefficients depend on the stepsize τ in time and – via r – on the dimension of the spatial discretization.

The implementation of the Chebyshev approximation is particularly efficient if the space is discretized using spectral methods based on Fourier–Galerkin or Fourier Collocation techniques [1, 3]. They allow the realization of each multiplication with H by means of two Fast Fourier Transforms reducing the asymptotic scaling of the computational effort of one matrix-vector multiplication to $d\, log_2(d)$ instead of d^2.

3 Error Estimation

It is our aim to estimate the global error which originates in the *numerical realization* of the Chebyshev approximation in comparison with the exact evolution operator. In this context, the term "global error" indicates the error accumulated during the total integration time from t_{initial} to t_{final}. Fortunately, the unitarity of our propagator effects that there is only accumulation but no amplification of discretization errors with time. Thus, if the *local error*, i.e., the error per time step, is bounded by some predefined local tolerance *tol* then we achieve an estimation of the global error:

$$\|\epsilon^{\text{global}}\| \leq k\, tol, \tag{8}$$

where k is the number of timesteps made. The global error is growing only linearly with the number of timesteps.
For this reason we might concentrate our further study on the local error analysis, i.e., on the discretization error introduced in one single time step, rather than on a global view.

To start with, one remark on the notation used: let us distinguish between any analytical quantity and its numerical realization by a tilde atop the latter. Thus, we denote the local error by

$$\epsilon = \exp(-i\, H_d\, \tau)\Psi_0 - \tilde{P}_N(r\tau\, H)\Psi_0,$$

where τ represents the length of the timestep. Obviously this error comprises two parts: The approximation error which measures the effect of the truncated expansion in Chebyshev polynomials and the round–off error which occurs in every numerical realization. This yields:

$$\epsilon = \epsilon_N + \epsilon_R,$$

with the approximation error:

$$\epsilon_N = \exp(-i\, H_d\, \tau)\Psi_0 - P_N(r\tau\, H)\Psi_0$$

and the round–off error:

$$\epsilon_R = P_N(r\tau\, H)\Psi_0 - \tilde{P}_N(r\tau\, H)\Psi_0.$$

In the following, we separately analyse both errors.

Approximation Error The approximation error can sufficiently be estimated via the Faber polynomial approximation theory [5, 6] because the Chebyshev polynomials are, up to a scalar factor, identical with certain Faber polynomials. One obtains the following result:

$$\begin{aligned} \|\epsilon_N\| &= \|\exp(-i\,H_d\,\tau)\Psi_0 \;-\; P_N(r\tau\,H)\Psi_0\| \\ &\le \frac{2}{1-\frac{r\tau}{N+1}}\left(\frac{e\,r\tau}{N+1}\right)^{N+1} \qquad (N+1\;>\;r\tau). \end{aligned} \tag{9}$$

The proof of this estimate is presented in [7]. According to it, ϵ_N exponentially decreases with increasing N if $re\tau < N$. Thus, analytically, for any stepsize τ any accuracy can be obtained by increasing N.

Stepsize Dependence of Round–Off Error The analysis of the round–off error ϵ_R can be based on a linearized error theory [8] in addition to the foundations of three–term recurrence relations ([9]; chapter 6 of [8]). The details of the investigation are collected in the appendix. They include the round–off error introduced by the recursion in order to compute the $\tilde{T}_k(r\tau\,H)\Psi_0$, by the evaluation of the coefficients c_k, and by the subsequent multiplication and summation yielding $\tilde{P}_N(r\tau\,H)\Psi_0$. The result is the following upper bound for the round–off error:

$$\begin{aligned} \|\epsilon_R\| &= \|P_N(r\tau\,H)\Psi_0 \;-\; \tilde{P}_N(r\tau\,H)\Psi_0\| \\ &\dot{\le} (\alpha_d\,(r\tau)^2 \;+\; \beta_d\,r\,\tau \;+\; \gamma_d)\,\mathrm{eps}, \end{aligned} \tag{10}$$

where eps denotes the machine precision. It is valid as long as the order N under consideration is "reasonably chosen", i.e., as long as it is not chosen foolishly large, e.g., much larger than those N with which the exponential decrease of the approximation error actually starts (cf. Fig. 2).

The result is reassuring because it guarantees that, for fixed space dimension, the total round–off error per time step increases only quadratically if the stepsize τ is increased. In contrast, many alternative polynomial expansions lead to a very strong, *successive amplification* of the round–off error. In many cases this amplification results in an *exponential* increase. For example, this is the case for the Taylor expansion (cf. Fig. (1)). Moreover, the Chebyshev expansion itself produces such exponential amplification if the spectrum of H becomes complex, i.e., in the case of dissipative quantum mechanics [7, 10] or if absorbing boundary conditions are applied [11].

By construction, this estimation reveals an *upper bound* for the round–off

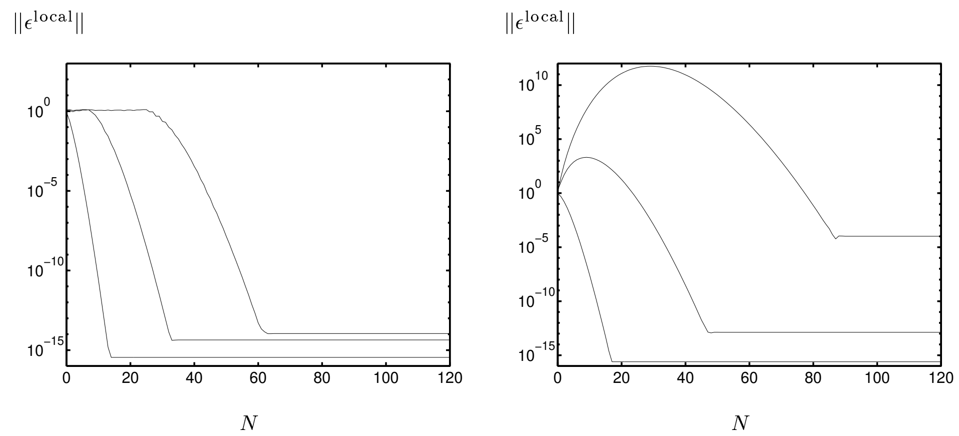

Figure 1: Dependence of the local error $||\epsilon^{\mathrm{local}}||$ on the approximation order N for the evaluation of $\exp(-i\tau A)$ for an hermitian 10×10 test matrix A for different stepsizes τ. The picture on the left hand side shows an approximation via Chebyshev polynomials, the picture on the right hand side an approximation via the truncated Taylor expansion. Obviously, the asymptotically remaining round–off error increases exponentially only in the second case.

error. Numerical simulations, to be presented in the next section, show that *the method is even better* than the upper bound promises: the actual dependence on the stepsize seems to be *linear*.

Grid Dependence of Round–Off Error The reader should also note, that the details of the estimation process disclose that the quantities α_d, β_d and γ_d of inequality (10) do not depend on τ but on the spatial dimension d! For a problem with one degree of freedom one finds that this dependence scales with the square root of d, i.e.,

$$\alpha_d,\, \beta_d,\, \gamma_d \,\propto\, d^{\frac{1}{2}}.$$

This is an effect of the numerical realization of the matrix–vector multiplication $H\Psi_0$ via Fast–Fourier–Transforms (FFT), which introduces a round–off error of scale $\mathcal{O}(d^{1/2})$ (see [12]). For larger numbers of degrees of freedom this d–dependence becomes even stronger.

Algorithmic Consequences At this point we are able to describe the consequences of the preceding results. Our opening question was whether the increase of the stepsize in time could threaten the reliability of the results of the simulation?

Obviously, for any given stepsize τ and with respect to the approximation error only, the Chebyshev expansion can realize any accuracy requirement for sufficiently large orders N: Assume a local tolerance $tol \geq$ eps to be given and choose N according to

$$\|\epsilon_N\| \quad \leq \quad \frac{2}{1-\frac{r\tau}{N+1}}\left(\frac{e\,r\tau}{N+1}\right)^{N+1} \leq tol.$$

While there is no restriction on the stepsize via the approximation error, it might come into play with the round–off error. First off all, the error estimate (10) leads to a lower bound for the possible tolerance $tol \geq \gamma_d\,\mathrm{eps}$. Let us therefore write the τ–dependence of the round–off error as:

$$\|\epsilon_R\| \mathrel{\dot{\leq}} (c_d\,(r\tau)^p + \gamma_d)\,\mathrm{eps}, \qquad (p \leq 2), \tag{11}$$

with some still d-dependent constant c_d. This formula summarizes our theoretical result ((10), $p = 2$) on one hand and the finding from numerical experiments ((cf. Fig. 3), $p = 1$) on the other. From the requirement $\|\epsilon_R\| < tol$, we obtain a restriction on the stepsize:

$$\tau \leq \sqrt[p]{\frac{1}{c_d\,r^p}\left(\frac{\mathrm{tol}}{\mathrm{eps}} - \gamma_d\right)}\,. \tag{12}$$

Herein, the constant c_d contains the d-dependence of the constants α_d and β_d from (10), i.e., for one degree of freedom

$$c_d \propto d^{1/2}, \quad \Rightarrow \quad c_d\,r^p \propto d^{2p+1/2}. \tag{13}$$

Thus, (12) is an important restriction for large spatial grid dimensions d:

$$\tau_{\max} \propto \frac{1}{d^{2+\frac{1}{2p}}}.$$

In the case of several degrees of freedom, the d dependence is even stronger and the restriction to τ even tougher.

Let us now return to the global view. Let the simulation interval in time be of length $T = t_{\text{final}} - t_{\text{initial}}$. Using a stepsize τ locally, we approximately have to make T/τ steps. According to (11) and (8), the global round–off error sums up to

$$\|\epsilon_R^{\text{global}}\| \le T\left(c_d T\,\tau^{p-1} + \frac{\gamma_d}{\tau}\right)\text{eps}.$$

Obviously, this estimate of the global round–off error has in the case of $p=1$ at $\tau = T$ a minimum which increases with d and T.

4 Numerical Results

In this section, the theoretical results are checked and illustrated by numerical simulations. Obviously, the requirement to analyse not only the approximation error but also the round–off error confines the possible examples to those, which can be solved with an extremely high precision. Therefore, we have chosen a simple model problem, an harmonic quantum oscillator, which is modeled to represent the ground state of an H–Cl molecule [13]. The Hamiltonian is given by:

$$H_{ex} = -\frac{\hbar^2}{2m}\Delta_x + \frac{m}{2}\omega^2 x^2. \tag{14}$$

The frequency of the oscillator corresponds to a wavenumber of 3000cm^{-1} or to an energy of $\hbar\omega = 35.78$ kJ/mol. The reduced mass of the H–Cl molecule is $m = 0.98u$.

We apply a Fourier collocation method as spatial discretization. The spatial discretization is, if not stated otherwise, done on a grid of 128 collocation points over a spatial computation domain $x/\text{Å} = [-4.2, 4.2]$.

The comparative solution is calculated with quadruple precision, i.e., eps $= 10^{-32}$, via the diagonalization of the matrix representation of the Hamilton operator. Note, that the introduction of a discrete grid and periodic boundary conditions prevent us from adopting the analytical solution of the harmonic quantum oscillator. The initial state was chosen to be a combination of some eigenstates of the discrete problem. Figure 2 shows the dependence of the local error $\|\epsilon^{\text{local}}\|$ on the approximation order N for different stepsizes τ = 41.3, 124.0, 206.7, 289.4, 372.1 fs.

As mentioned before, the local error comprises two parts: the approximation error ϵ_N and the round–off error ϵ_R. The results reflect the expected exponential decay of the approximation error with growing approximation order N. But obviously, the error does not reach machine precision (herein eps=$2\cdot 10^{-16}$), even for great N. We observe an asymptotically remaining,

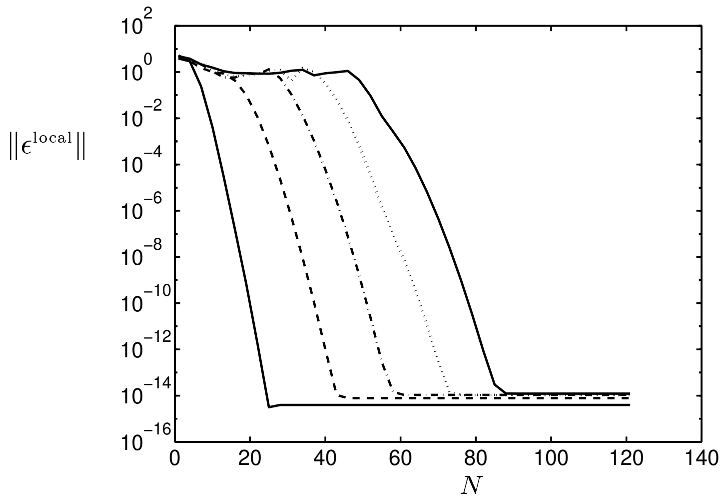

Figure 2: Dependence of the local error $\|\epsilon^{\text{local}}\|$ on the approximation order N for different stepsizes . $\tau = 41.3$ fs (left solid line), $\tau = 124.0$ fs (dashed line), $\tau = 206.7$ fs (dashed–dotted line), $\tau = 289.4$ fs (dotted line), $\tau = 372.1$ fs (right solid line)

τ–depending error, which is almost independent of N. It can be connected with the round–off error: For N large enough, we have $\|\epsilon_N\| \ll \|\epsilon_R\|$ which implies $\|\epsilon^{\text{local}}\| \approx \|\epsilon_R\|$. This observation of a nearly constant remainder illustrates the theoretical result (10) which gives us an upper bound for the round–off error which is independent from N. For a closer examination of the round–off error we analysed the dependence of this remaining local error on the stepsize τ (cf. Figure 3). The reader should note the linear growth in τ which verifies our theoretical estimation of the round–off error but promises an even better numerical stability of the Chebyshev method. This observation corresponds to the case $p = 1$ in (11) with all the consequences discussed above.

But note, the linearity of growth of the asymptotically remaining local error can also be a result of a small constant in front of the quadratic term in (10). This would mean, that for very large stepsizes in time, there might be a quadratic increase.

Finally we are interested in the dependence of the round–off error, i.e., the remainder for great N, on the spatial dimension d. Figure 4 illustrates the results using an uniform timestep $\tau = 4.1$ fs and a variety of spatial dimensions. Note that the regression line in the double logarithmic representation has a gradient of 2.4. Thus we obtain a round–up error proportional to $d^{2.4}$

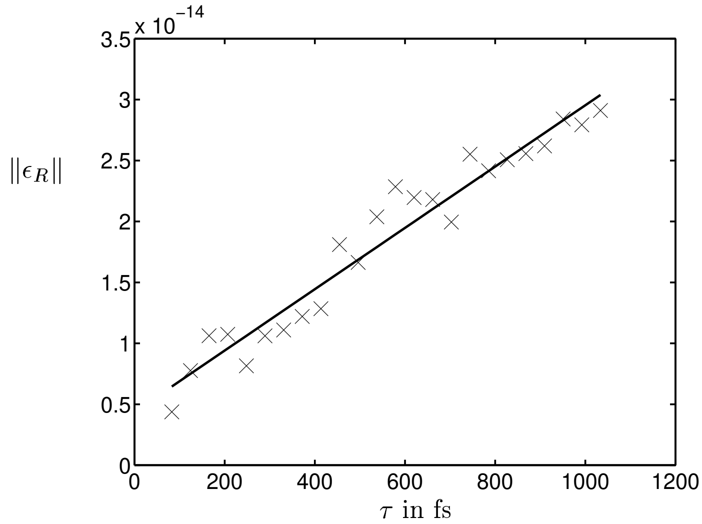

Figure 3: Dependence of the asymptotically remaining local error, i.e., round–off-error $\|\epsilon_R\|$, on the stepsize τ in time.

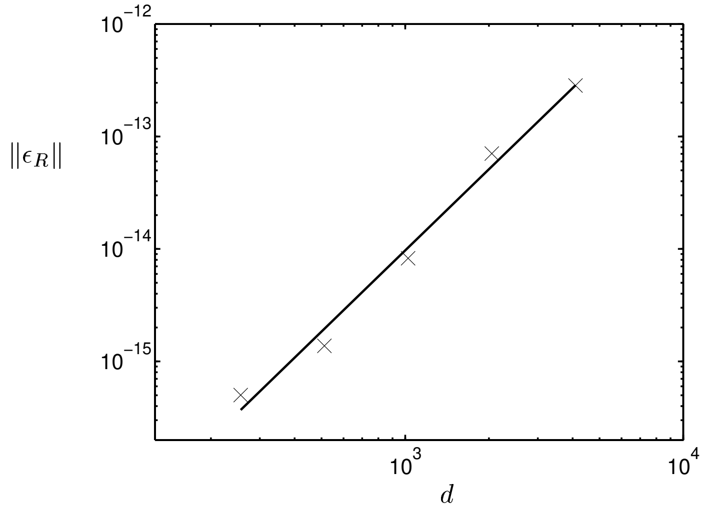

Figure 4: Dependence of the round–off-error $\|\epsilon_R\|$ on the spatial dimension d.

which fits the theoretical result (13) for $p = 1$.

Conclusively, all observations perfectly reflect the theoretical results.

Appendix

In this section the proofs and details of the estimate (10) of the round–off error are presented. As the reader might remember we denoted the *analytic* Chebyshev approximation of the solution $\Psi(\tau) = \exp(-i\tau H)\Psi_0$ of (2) by

$$P_N(r\tau H)\Psi_0 \;=\; \sum_{k=0}^{N} c_k(r\tau)\, T_k(H)\Psi_0,$$

with short notation $P_N\Psi_0$. We are interested in its *numerical* realization $\tilde{P}_N(r\tau H)$ or, more exactly, in the round–off error

$$\epsilon_R(N, r\tau) \;=\; \tilde{P}_N(r\tau H)\Psi_0 \;-\; P_N(r\tau H)\Psi_0$$

of the Chebyshev approximation, which depends on the machine precision eps . The numerical error consists of three different parts:

1. The computation of the coefficients $c_k(r\tau)$ via the Bessel functions.

2. The evaluation of all the $T_k(H)\Psi_0$ via the recursion of the Chebyshev polynomials and the FFT–algorithm.

3. The successive summation.

Below we will present estimates for each of the three parts using linearized round–off error analysis [8].

4.1 The computation of the Bessel functions

Herein, we will assume that, either, the computation of the c_k is not necessary because they are available via table look–up, or, that their evaluation is as precise as an elementary operation. In other words, the computed values $\tilde{c}_k$ are assumed to be of the form

$$\tilde{c}_k \;=\; c_k \;+\; \Delta c_k \doteq c_k\,(1 + \alpha_k\,\mathrm{eps}), \tag{15}$$

with $|\alpha_k| < 1$, i.e., the Δc_k are of order eps.

4.2 The computation of the Chebyshev polynomials

The following argumentation is comparable to a condition analysis in [8] or [9].

We will estimate the error which results from the numerical realization $\tilde{T}_{k+1}\,\Psi_0$ of the Chebyshev polynomial T_{k+1} applied on Ψ_0:

$$\Delta T_{k+1}(H)\Psi_0 \;=\; \tilde{T}_k(H)\Psi_0 \;-\; T_k(H)\Psi_0.$$

Let us skip the argument H of the Chebyshev polynomials in the following. Due to our restriction to a linearized error analysis we might write the realized three–term recursion in the following way:

$$\tilde{T}_{k+1}\Psi_0 \doteq (\mathrm{Id} + \beta_{k+1}\,\mathrm{eps})\Big((\mathrm{Id} + \Gamma^d_{k+1}\,\mathrm{eps})\,2H\tilde{T}_k\Psi_0 \;-\; \tilde{T}_{k-1}\Psi_0\Big)$$

with diagonal matrices Γ^d_{k+1} and β_{k+1} corresponding to the application of the Hamilton operator on $\tilde{T}_k\Psi_0$ respectively the summation. Because β_{k+1} represents an elementary operation, it is bounded by one. The reader should note that Γ^d_{k+1} depends crucially on the spatial dimension via the FFT algorithm.

We derive easily:

$$\tilde{T}_{k+1}\Psi_0 \doteq \Big(\mathrm{Id} + (\Gamma^d_{k+1} + \beta_{k+1})\mathrm{eps}\Big)\,2H\tilde{T}_k\Psi_0 \;-\; (\mathrm{Id} + \beta_{k+1}\,\mathrm{eps})\tilde{T}_{k-1}\Psi_0,$$

which leads us to a perturbed recursion for the error $\Delta T_{k+1}\Psi_0$:

$$\begin{aligned}
\Delta T_{k+1}\Psi_0 \;&\doteq\; \Big(\mathrm{Id} + (\Gamma^d_{k+1} + \beta_{k+1})\mathrm{eps}\Big)\,2H\,\tilde{T}_k\,\Psi_0 \\
&\quad - (\mathrm{Id} + \beta_{k+1}\,\mathrm{eps})\,\tilde{T}_{k-1}\Psi_0 \;-\; \Big(2HT_k\Psi_0 \;-\; T_{k-1}\Psi_0\Big) \\
&\doteq\; 2H\Delta T_k\Psi_0 \;-\; \Delta T_{k-1}\Psi_0 + E_{k+1}\Psi_0
\end{aligned} \tag{16}$$

with

$$E_{k+1} \doteq ((\Gamma^d_{k+1} + \beta_{k+1})\mathrm{eps})\,2H\tilde{T}_k \;+\; (\beta_{k+1}\,\mathrm{eps})\,\tilde{T}_{k-1}$$

and the initial values $\Delta T_1\,\Psi_0 \;=\; (\Gamma^d_{k+1}\mathrm{eps})\;H\Psi_0$ and $\Delta T_0\Psi_0 \;=\; 0$.

The solution of (16) is given by:

$$\Delta T_k(H) \;=\; \sum_{j=0}^{k} E_j U_{k-j}(H)$$

where U_j is the jth Chebyshev polynomial of the second kind.

Using $\rho(H) < 1$ we get an upper bound for the norm of $U_m(H)$:

$$\|U_m(H)\| \;=\; \sup_{\lambda\in\sigma(H)}\{U_m(\lambda)\} \;<\; \frac{2}{1-\rho(H)^2} \;=:\bar{U}. \tag{17}$$

Note, that in (17) it is of prime importance to guarantee that the spectral radius does actually not reach unity (cf. (3)).

Using $\|\tilde{T}_k(H)\| < 1$ we can estimate E_{k+1} by:

$$
\begin{aligned}
\|E_{k+1}\| &\leq 2\|H\|\,\|\tilde{T}_k\|\,(|\Gamma^d_{k+1}| + |\beta_{k+1}|)\text{eps} + \|\tilde{T}_{k-1}\|\,|\beta_{k+1}|\,\text{eps} \\
&\leq (2|\Gamma^d_{k+1}| + 3|\beta_{k+1}|)\,\text{eps} \\
&\leq \bar{E}^d\,\text{eps} \qquad (18)
\end{aligned}
$$

with the constant $\bar{E}^d = \max_{k\leq N-1}\{(2|\Gamma^d_{k+1}| + 3|\beta_{k+1}|)\}$.

Combining (17) and (18) we find an upper bound for the error of the numerical realization of the Chebyshev polynomials:

$$
\begin{aligned}
\|\Delta T_k(H)\,\Psi_0\| &\leq \sum_{j=0}^{k} \|E_j\|\,\|U_{k-j}(H)\| \\
&< \bar{E}^d\,\bar{U}\sum_{j=0}^{k}\text{eps} \\
&= C^d\,(k+1)\,\text{eps}. \qquad (19)
\end{aligned}
$$

with a constant $C^d > 0$ strongly depending on the spatial dimension d.

4.3 The summation process

With these two results we are able to investigate the summation process. Let $\tilde{P}_{k-1}\Psi_0$ denote the computed value of the $(k-1)$th Chebyshev approximation. Then, the kth is evaluated as the product of the two floating point results $\tilde{c}_k$ and $\tilde{T}_k(H)\Psi_0$ added to the vector $\tilde{P}_{k-1}\Psi_0$. Herein, summation and multiplication are floating point operations, i.e.,

$$
\tilde{P}_k\Psi_0 \doteq (\mathrm{Id} + \beta_\mathrm{k}\,\mathrm{eps})\,\Big(\tilde{\mathrm{P}}_{\mathrm{k}-1}\Psi_0 + (\mathrm{Id} + \gamma_\mathrm{k}\,\mathrm{eps})\,\tilde{\mathrm{c}}_\mathrm{k}\,\tilde{\mathrm{T}}_\mathrm{k}(\mathrm{H})\Psi_0\Big)
$$

with diagonal matrices β_k, γ_k and $\|\beta_k\|, \|\gamma_k\| < 1$. Due to the linear error concept a direct evaluation leads to the following recursion for the round–off error after k steps:

$$
\begin{aligned}
\epsilon_R(k, r\tau) \doteq\ & \epsilon_R(k-1, r\tau) + c_k\,\Delta T_k(H)\Psi_0 + \beta_k\,P_{k-1}\Psi_0\,\text{eps} \\
& + \Delta c_k\;T_k(H)\Psi_0 + (\beta_k + \gamma_k)\,c_k\,T_k(H)\Psi_0\;\text{eps}.
\end{aligned}
$$

Thus, with suitable values for ΔT_0, Δc_0, γ_0 and β_0 and the Δc_k from (15), we have

$$\begin{aligned}\epsilon_R(k, r\tau) &\doteq \sum_{k=0}^{N} c_k \; \Delta T_k(H)\Psi_0 \, \mathrm{eps} + \sum_{k=1}^{N} \beta_k \, P_{k-1}\Psi_0 \, \mathrm{eps} \\ &\quad + \sum_{k=0}^{N} (\alpha_k \mathrm{Id} + \mathrm{\beta_k} + \mathrm{\gamma_k}) \; \mathrm{c_k} \; \mathrm{T_k(H)}\Psi_0 \; \mathrm{eps}.\end{aligned}$$

Below, we will give estimates for each of the three summands. Easily, we get:

$$\begin{aligned}\| \sum_{k=0}^{N} (\alpha_k \mathrm{Id} + \beta_k + \gamma_k) \; c_k \; T_k(H)\Psi_0 \| &< 3 \sum_{k=0}^{N} |c_k| \\ \| \sum_{k=0}^{N} c_k \; \Delta T_k(H)\Psi_0 \| &< C^d \sum_{k=0}^{N} (k+1)\, |c_k|,\end{aligned}$$

while the second one gives us – via a rearrangement of the two sums –

$$\| \sum_{k=1}^{N} \beta_k \, P_{k-1}\Psi_0 \, \| = \| \sum_{k=0}^{N-1} \left(\sum_{l=k+1}^{N} \beta_l \right) \; c_k \; T_k(H)\Psi_0 \| < \sum_{k=0}^{N-1} (N-k)\, |c_k|.$$

We now present two different approaches to provide an estimate for the round–up error, which differ in handling the expansion coefficients c_k. While the effort in applying these approaches differs a lot, there is no substantial change in the result. The first approach bounds every $|c_k(r\tau)|$ with 2, which is clearly an upper bound but for $k \geq r\tau$ a rough overestimation (cf. Figure 5). Nevertheless we get:

$$\begin{aligned}\|\epsilon_R\| &\dot{<} \left(3 \sum_{k=0}^{N} |c_k| \; + \; C \sum_{k=0}^{N} (k+1)\, |c_k| \; + \; \sum_{k=0}^{N-1} (N-k)\, |c_k| \right) \mathrm{eps} \\ &\dot{<} \left((C+1)\, N^2 \; + \; (3\, C + 7)\, N \; + \; (2\, C + 6) \right) \mathrm{eps}. \qquad (20)\end{aligned}$$

We are interested in an approximation error $\epsilon_A(N)$ smaller than some predefined tolerance *tol*. It is easy to show that there exists an $m \geq 1$, only depending on *tol*, so that we find an

$$r\,\tau < N < m\, r\tau \qquad (21)$$

with $\epsilon_A(N) \leq tol$. Thus, we may restrict ourselves to those suitable choices of N. Obviously, inserting (21) into (20) yields a quadratic growth in $r\tau$.

For the second approach we use an improved estimate for the asymptotic decrease of the c_k. According to [14] an upper bound for the Bessel–functions and, thus, the c_k is given by

$$|c_k(r\tau)| \;=\; |2\,J_k(r\tau)| \;\leq\; 2\,\min\{1,\,\frac{|(r\tau)/2|^k}{(k+1)!}\} \qquad\qquad k \geq 1.$$

Figure 5 illustrates the decrease of the exact coefficients and our upper bound. Calculations basing on this estimation yields a quadratic growth in $r\tau$ as well.

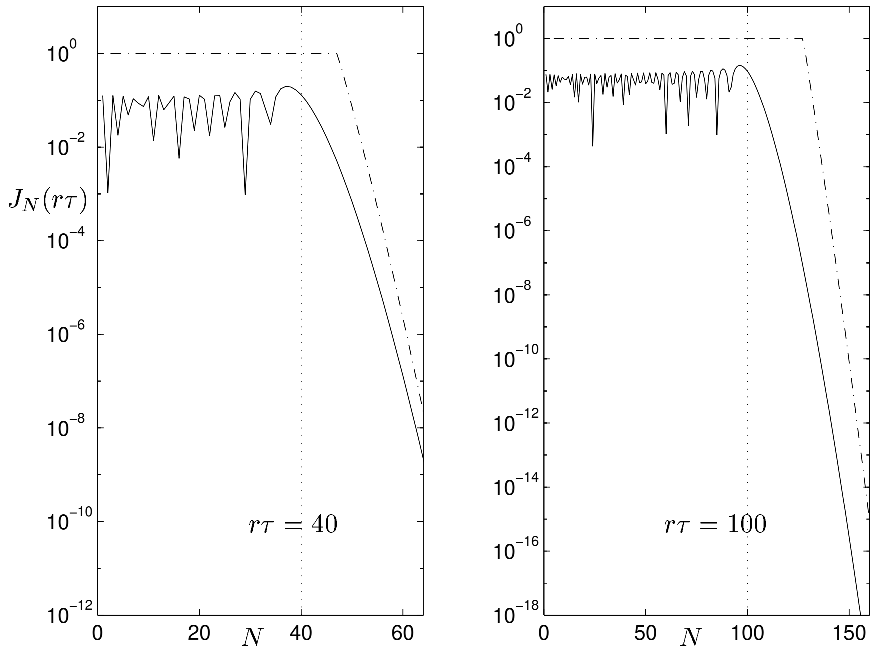

Figure 5: Decay of the coefficients $c_N(r\tau)/2$ (solid line) and the upper bound (dashed line) with N for fixed $r\tau = 40$ (left hand side) and $r\tau = 100$ (right hand side).

Collecting the preceding results yields the following statement:

Lemma 4.1 *In the context of linear error theory the round–off error of the realization of the Chebyshev approximation on a computer with machine precision eps can be estimated by*

$$\|\epsilon_R\| < \Big(\alpha_d\,(r\tau)^2 + \beta_d\, r\,\tau + \gamma_d\Big)\;eps, \tag{22}$$

where $\alpha_d, \beta_d, \gamma_d$ are constants regarding N and $r\tau$.

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