The direct midpoint method as a quantum mechanical integrator II *

Ulrich Mutze †

A reversible integrator for the time-dependent Schrödinger equation associated with an arbitrary (potentially time-dependent) Hamilton operator is defined. This algorithm assumes the dynamical state of the system to be described by a conventional quantum state vector and a velocity vector of the same data structure and storage size. The algorithm updates these two vectors by five additions of vectors, three multiplications of vectors with real numbers, and four actions of the Hamilton operator on a vector. If the Hamilton operator is time-independent, additions of vectors reduce to three, and the actions of the Hamilton operator reduce to one action of its square. In the first of a series of steps, the velocity has to be initialized by one action of the Hamilton operator on the initial state vector. Further properties of this algorithm are derived only for finite dimensional state spaces and time-independent Hamilton operators. Under these assumptions it is shown that the time step evolution operator is symplectic so that exact energy conservation holds. Further, an explicit expression for the n-th power of the time step evolution operator is derived. This makes the system behavior completely transparent: There is a limiting time step, namely 2 divided by the norm of the Hamilton operator, so that for smaller time steps all trajectories remain bounded for all times, whereas for larger time steps there are always exponentially growing trajectories. For time steps smaller than the limit there is approximate conservation of norm along each trajectory and the deviation from exact conservation is controlled by explicit expressions proportional to the square of the time step.

1 Introduction

This paper is about a method for solving the numerical initial value problem of the time-dependent Schrödinger equation with time-independent Hamiltonian. In order

*updated version of the theoretical part of [11]

†ulrichmutze@aol.com

to see how the method arises and what its particularities are, it is useful to start with a more general problem, which is common to quantum mechanics, electrodynamics, and linear systems engineering. We thus consider the differential equation

$$\dot{\psi}(t) = D(t)\,\psi(t) + f(t) \tag{1}$$

for a time-dependent quantity ψ which takes values in a real vector space $\mathcal{H}$ and which is under control of a $\mathcal{H}$-valued function f, and a function D, the values of which are linear operators $\mathcal{H} \to \mathcal{H}$.

A useful computational solution of the initial value problem of first-order differential equations is provided by the *leap-frog method* or *explicit midpoint rule* which for our equation may be written as

$$\psi(t+\tau) := \psi(t-\tau) + 2\tau\,(D(t)\,\psi(t) + f(t))\ . \tag{2}$$

If we are given $\psi(t_0)$, this *two-step method* cannot start directly since we need to know $\psi(t_0+\tau)$ too. This value may be provided by the *explicit Euler rule*

$$\psi(t_0+\tau) := \psi(t_0) + \tau\,(D(t_0)\,\psi(t_0) + f(t_0))\ . \tag{3}$$

It is convenient to transform this into a *one-step method* in such a manner that it becomes possible to change the time increment τ after each step. The definitions

$$\phi(t+\tau) := \frac{\psi(t+\tau)-\psi(t)}{\tau}\ , \quad \phi(t-\tau) := \frac{\psi(t)-\psi(t-\tau)}{\tau}\ , \quad \phi(t) := \frac{\phi(t+\tau)+\phi(t-\tau)}{2} \tag{4}$$

allow rewriting (2) as

$$\phi(t) = D(t)\,\psi(t) + f(t) \tag{5}$$

and computing the quantities $\psi(t+\tau), \phi(t+\tau)$ from $\psi(t-\tau), \phi(t-\tau)$, where $\psi(t), \phi(t)$ appear as temporaries:

$$\begin{aligned} \psi(t) &:= \psi(t-\tau) + \tau\phi(t-\tau)\ , \\ \phi(t) &:= D(t)\,\psi(t) + f(t)\ , \\ \phi(t+\tau) &:= 2\phi(t) - \phi(t-\tau)\ , \\ \psi(t+\tau) &:= \psi(t) + \tau\phi(t+\tau)\ . \end{aligned} \tag{6}$$

In the first step of a series of integration steps we are given $\psi(t_0)$ and define

$$\phi(t_0) := D(t_0)\,\psi(t_0) + f(t_0) \tag{7}$$

which then is sufficient to compute the next ψ,ϕ-pair from (6). This suggests the following definition of a *modified leap-frog integrator* for the differential equation (1): For each

$h \in \mathbb{R}$ we define

$$\begin{aligned}
\Gamma_h &: \mathbb{R} \times \mathcal{H} \times \mathcal{H} \to \mathbb{R} \times \mathcal{H} \times \mathcal{H} \,, \\
\Gamma_h(t,\psi,\phi) &:= (\underline{t},\underline{\psi},\underline{\phi}) \quad \text{where} \\
\tau &:= \frac{h}{2} \,, \\
t' &:= t + \tau \,, \\
\psi' &:= \psi + \tau\phi \,, \\
\phi' &:= D(t')\,\psi' + f(t') \,, \\
\underline{t} &:= t' + \tau \,, \\
\underline{\phi} &:= 2\phi' - \phi \,, \\
\underline{\psi} &:= \psi' + \tau\underline{\phi} \,.
\end{aligned} \tag{8}$$

Obviously Γ_0 is the identity map, and Γ is *reversible* in the sense that for all $h \in \mathbb{R}$ we have

$$\Gamma_{-h} \circ \Gamma_h = \Gamma_0 \,. \tag{9}$$

This property has been made possible by the introduction of ϕ as a part of the state description: Consider a discrete trajectory

$$s_0 := (t_0, \psi_0, \phi_0),\ s_1 := \Gamma_{h_1} s_0 \,,\ \ldots \,,\ s_n := \Gamma_{h_n} s_{n-1} \,, \quad \text{where} \quad \phi_0 := D(t_0)\psi_0 + f(t_0) \,, \tag{10}$$

then the final state s_n contains the information that is needed to go the way exactly back to the initial state. Actually, equation (9) implies

$$s_{n-1} = \Gamma_{-h_n} s_n \,,\ \ldots \,,\ \Gamma_{-h_1} s_1 = s_0 \,.$$

Neglecting the ϕ-component of state s_n and setting it from the ψ-component — just as (10) treated the initial state s_0 — allows reaching ψ_0 only approximately.

Iterating mappings Γ_h generates discrete trajectories from arbitrary initial states $(\psi_0, \phi_0) \in \mathcal{H} \times \mathcal{H}$. Dependent on how large the difference $\delta(t_0) := \phi_0 - D(t_0)\,\psi_0 - f(t_0)$ is, these trajectories may not be reasonable approximations to trajectories of the differential equation (1). They then are zig-zag lines which tend to wiggle around such trajectories. Also for trajectories which start with $\delta(t_0) = 0$, all the following $\delta(t_i)$ will slightly differ from 0 since the step algorithm enforces (5) only for the hidden midpoint states.

The role of the state component ϕ is to memorize the state of the previous step in a format which is independent of the point in time to which this previous state belonged. The generic transformations from multi-step methods to one-step methods considered in numerical mathematics (e.g. [6] Section 3.5.4) don't achieve this hiding of the previous step size and thus don't allow changing the time increment from step to step. Further, they don't suggest a concept of reversibility. The quantity ϕ thus seems to be indispensable as a component of the computational state if a simple and reversible integrator is to operate on those computational states. By contrast, the non-discretized

system as defined by the first order differential equation (1) needs no state data in addition to ψ. This suggests the basic idea of the present method: to harmonize the mathematical and the computational treatment by modifying the differential equation in a manner that it determines the evolution of ψ,ϕ-pairs. This is, of course, implemented by considering the differential equation which results from (1) by differentiation:

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix}\psi(t)\\ \phi(t)\end{pmatrix} = \begin{pmatrix}\phi(t)\\ F(\psi(t),t)\end{pmatrix}, \tag{11}$$

where

$$F(\psi(t),t) := D(t)\,(D(t)\,\psi(t)+f(t)) + \dot{D}(t)\,\psi(t) + \dot{f}(t)\,. \tag{12}$$

Now, ψ and ϕ are components of a quantity which evolves in time according to the differential equation (11) and the initial value problem of this equation assumes $\psi(t_0)$ and $\phi(t_0)$ to be given. If these quantities are related as in (7), then the trajectory of (11) with these initial values is also a trajectory of (1) with initial value $\psi(t_0)$.

Equations of type (11) arise in classical mechanics: Interpreting ψ as a collection of particle coordinates and ϕ as a collection of particle momenta, we may interpret (11) as equations of motion for particles which move under the influence of forces F that depend only on positions and not on momenta. For such classical equations of motion many integrators have been studied. Experience with computationally expensive systems comes from celestial mechanics, molecular dynamics, and the dynamics of granular media.

A family of powerful integrators builds on the basic algorithmic idea in [1]. A particularly symmetric member of this family is the *position Verlet integrator* introduced in [4]. An equivalent integrator is discussed in [5] as the *explicit partitioned Runge-Kutta method* charcterized by the tableaux $(0,1)[1/2,1/2]$. A further equivalent integrator, which also applies to velocity dependent forces, has been derived from a one-step variational principle in [10], where the name *direct midpoint method* is proposed for this specific form, in analogy to the name *explicit midpoint method* of the closely related leap-frog method. Also the original Verlet algorithm is related to a discrete variational principle, see [8].

Applied to (11) in the mechanical interpretation the position Verlet integrator is given as follows

$$\begin{aligned}
\tau &:= \frac{h}{2}\,, \quad t' := t+\tau\,, \quad \underline{t} := t'+\tau\,,\\
\psi' &:= \psi + \tau\phi\,,\\
\underline{\phi} &:= \phi + hF(\psi',t')\,,\\
\underline{\psi} &:= \psi' + \tau\underline{\phi}\,.
\end{aligned} \tag{13}$$

When applied to F from (12), this is not completely explicit due to the terms $\dot{D}$ and $\dot{f}$ in F. We thus replace these terms by suitable symmetric differences

$$\dot{D}(t') = \frac{D(\underline{t})-D(t)}{h} + O(h^2)\,, \quad \dot{f}(t') = \frac{f(\underline{t})-f(t)}{h} + O(h^2) \tag{14}$$

so that the term $hF(\psi',t')$ changes to

$$hD(t')\left(D(t')\psi'+f(t')\right)+D(\underline{t})\psi'+f(\underline{t})-D(t)\psi'-f(t)\,.$$

This allows us to define the *direct midpoint integrator* for the present context in close analogy to (8) as follows:

$$\begin{aligned}
\tilde{\Gamma}_h &: \mathbb{R}\times\mathcal{H}\times\mathcal{H}\to\mathbb{R}\times\mathcal{H}\times\mathcal{H}\,,\\
\tilde{\Gamma}_h(t,\psi,\phi) &:= (\underline{t},\underline{\psi},\underline{\phi}) \quad \text{where}\\
\tau &:= \frac{h}{2}\,,\\
t' &:= t+\tau\,,\\
\psi' &:= \psi+\tau\phi\,,\\
\underline{t} &:= t'+\tau\,,\\
\underline{\phi} &:= \phi+hD(t')\left(D(t')\psi'+f(t')\right)+D(\underline{t})\psi'+f(\underline{t})-D(t)\psi'-f(t)\,,\\
\underline{\psi} &:= \psi'+\tau\underline{\phi}\,.
\end{aligned} \tag{15}$$

Also this integrator is easily seen to be reversible. Its symmetry is best expressed in an algorithmic form which allows changing values of quantities without changing their name: Changing the time by 2τ induces a state change given by

$$\begin{aligned}
t &+= \tau\\
\psi &+= \tau\phi\\
\phi &+= 2\tau D(t)\left(D(t)\psi+f(t)\right)+D(t+\tau)\psi+f(t+\tau)-D(t-\tau)\psi-f(t-\tau)\\
\psi &+= \tau\phi\\
t &+= \tau\,.
\end{aligned} \tag{16}$$

Here, of course, $a \mathrel{+}= b$ means that a is to be changed to $a+b$. In quantum mechanical applications we have $f=0$. This algorithm was proposed in [10], equation (86), with the terms $D(t+\tau)\psi$ and $D(t-\tau)\psi$ missing. These terms are essential for good accuracy for strongly time-dependent Hamilton operators. The observations concerning restoration of norm and energy which are reported there find their explanations in the results of Subsection 2.2, particularly in equations (55) and (61), see also the remark following (31).

2 The direct midpoint integrator for the Schrödinger equation

From now on, let $\mathcal{H}$ be a complex Hilbert space of finite dimension d, D a skew-symmetric linear operator in $\mathcal{H}$, and $H := \mathrm{i}D$, which then is a symmetric operator. Even if we started with a skew-symmetric operator in a real Hilbert space — a situation which naturally arises in computational electrodynamics — one can always achieve this situation by means of complexification.

The time-dependent Schrödinger equation

$$\dot{\psi}(t) = D\psi(t) \tag{17}$$

is a special case of (1) and equation (11) simplifies to

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix}\psi(t)\\ \phi(t)\end{pmatrix} = \begin{pmatrix}\phi(t)\\ D^2\psi(t)\end{pmatrix} = \begin{pmatrix}0 & 1\\ D^2 & 0\end{pmatrix}\begin{pmatrix}\psi(t)\\ \phi(t)\end{pmatrix} . \tag{18}$$

We endow the space $\mathcal{H}\times\mathcal{H}$ in (15) with the structure of a Hilbert space by identifying it with the orthogonal sum $\mathcal{H}_d := \mathcal{H}\oplus\mathcal{H}$ and employ a natural matrix notation for linear operators in this space. The elements of $\mathcal{H}_d$ are referred to as *dynamical states* and are written in any of the notations $\begin{pmatrix}\psi\\ \phi\end{pmatrix}$ or (ψ,ϕ) or $\psi\oplus\phi$ if the components with respect to the decomposition of $\mathcal{H}_d$ are to be displayed. The exact solution of the initial value problem is

$$\begin{pmatrix}\psi(t)\\ \phi(t)\end{pmatrix} = \exp(t\,D_{\mathrm{mix}})\begin{pmatrix}\psi(0)\\ \phi(0)\end{pmatrix} , \quad \text{where} \quad D_{\mathrm{mix}} := \begin{pmatrix}0 & 1\\ D^2 & 0\end{pmatrix} . \tag{19}$$

The structure of D_{mix} makes it easy to re-arrange its exponential series and to obtain

$$\exp(t\,D_{\mathrm{mix}}) = \begin{pmatrix}\cosh(tD) & t\,\mathrm{sinch}(tD)\\ D\sinh(tD) & \cosh(tD)\end{pmatrix} , \tag{20}$$

where $\mathrm{sinch}(x) := \sinh(x)/x$. Since D_{mix} is not skew-symmetric, $\exp(t\,D_{\mathrm{mix}})$ is not unitary. However, D_{mix} is skew-symmetric with respect to the natural *symplectic form*

$$\Omega(\psi_1\oplus\phi_1,\psi_2\oplus\phi_2) := \langle\,\psi_1\,|\,\phi_2\,\rangle - \langle\,\phi_1\,|\,\psi_2\,\rangle , \tag{21}$$

so that $\exp(t\,D_{\mathrm{mix}})$ is symplectic (i.e. it leaves Ω invariant). This implies

$$\Omega(\psi(t)\oplus\phi(t),\psi(t)\oplus\phi(t)) = \Omega(\psi(0)\oplus\phi(0),\psi(0)\oplus\phi(0)) ,$$

thus

$$\langle\,\psi(t)\,|\,\phi(t)\,\rangle - \langle\,\phi(t)\,|\,\psi(t)\,\rangle = \langle\,\psi(0)\,|\,\phi(0)\,\rangle - \langle\,\phi(0)\,|\,\psi(0)\,\rangle ,$$

and

$$\Im\langle\,\psi(t)\,|\,\phi(t)\,\rangle = \Im\langle\,\psi(0)\,|\,\phi(0)\,\rangle . \tag{22}$$

The real part of this quantity needs not to be constant and (18) implies

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\,\psi(t)\,|\,\psi(t)\,\rangle = 2\,\Re\langle\,\psi(t)\,|\,\phi(t)\,\rangle . \tag{23}$$

So far, we have considered consequences of (18) and have ignored (17). The solutions of (7) now give rise to a linear space $\mathcal{H}_0 := \{(\psi,\phi)\,:\,\psi\in\mathcal{H},\,\phi = D\psi\}\subset\mathcal{H}_d$ of those dynamical states for which trajectories of (18) and of (17) are related in the manner described

in Section 1 in the sequel of equation (12) for the more general equations considered there. The subspace $\mathcal{H}_0$ is easily seen to be invariant under D_{mix} and, obviously, also under

$$D_{\mathrm{diag}} := \begin{pmatrix} D & 0 \\ 0 & D \end{pmatrix} . \tag{24}$$

Although D_{mix} and D_{diag} look rather different, they coincide when restricted to $\mathcal{H}_0$. Therefore, also the unitary operator $\exp\left(t\, D_{\mathrm{diag}}\right)$ coincides on $\mathcal{H}_0$ with the symplectic operator $\exp\left(t\, D_{\mathrm{mix}}\right)$. This can also be seen from the following explicit formula

$$\exp\left(t\, D_{\mathrm{mix}}\right) = \exp(t\, D_{\mathrm{diag}}) + \begin{pmatrix} -\sinh\left(tD\right) & t\,\mathrm{sinch}\left(tD\right) \\ D\sinh\left(tD\right) & -\sinh\left(tD\right) \end{pmatrix} , \tag{25}$$

which follows from (20).

We now study the integrator (15) for the present special case. The algorithm (16) specializes to

$$\begin{aligned} \psi \mathrel{+}= & \frac{h}{2}\,\phi \\ \phi \mathrel{+}= & \, h D^2\, \psi \\ \psi \mathrel{+}= & \frac{h}{2}\,\phi\,, \end{aligned} \tag{26}$$

and the obvious decomposition of (26) into three steps can be written as a composition of linear maps:

$$\begin{pmatrix} \underline{\psi} \\ \underline{\phi} \end{pmatrix} = \begin{pmatrix} 1 & \frac{h}{2} \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ hD^2 & 1 \end{pmatrix} \begin{pmatrix} 1 & \frac{h}{2} \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \psi \\ \phi \end{pmatrix} =: U_h \begin{pmatrix} \psi \\ \phi \end{pmatrix} . \tag{27}$$

These factors are easily seen to be symplectic. Thus U_h too is symplectic; it may be written as

$$U_h = \begin{pmatrix} 1+\frac{h^2}{2}D^2 & h(1+\frac{h^2}{4}D^2) \\ hD^2 & 1+\frac{h^2}{2}D^2 \end{pmatrix} = \begin{pmatrix} 1-\frac{h^2}{2}H^2 & h(1-\frac{h^2}{4}H^2) \\ -hH^2 & 1-\frac{h^2}{2}H^2 \end{pmatrix} = \exp\left(h D_{\mathrm{mix}}\right) + O(h^3)\,. \tag{28}$$

Notice that, unlike $\exp\left(h D_{\mathrm{mix}}\right)$, the operator U_h does not leave the subspace $\mathcal{H}_0$ exactly invariant. Together with U_h, all powers

$$U_h^n := (U_h)^n \tag{29}$$

are symplectic operators which implies energy conservation along each trajectory which is created by applying U_h iteratively on a dynamical state in $\mathcal{H}_0$. Considering

$$s_0 := (\psi, D\psi),\;\; s_1 := U_h s_0 = (\psi_h^1, \phi_h^1),\;\; s_2 := U_h s_1 = (\psi_h^2, \phi_h^2),\;\; \ldots \tag{30}$$

we have for each $n \in \mathbb{N}$

$$2\Im\langle\, \psi_h^n \,|\, \phi_h^n \,\rangle = \Omega(s_n, s_n) = \Omega(s_0, s_0) = 2\Im\langle\, \psi \,|\, D\psi \,\rangle = -2\langle\, \psi \,|\, H\psi \,\rangle\,. \tag{31}$$

Note that the quantity $-\Im\langle\psi_h^n|\phi_h^n\rangle$, although it is constantly equal to $\langle\psi|H\psi\rangle$, equals $\langle\psi_h^n|H\psi_h^n\rangle$ only approximately. In ignorance of (31) one may monitor $\langle\psi_h^n|H\psi_h^n\rangle$ as a test for energy conservation along a trajectory and will find it wiggling around some magical constant value — the constant value of $-\Im\langle\psi_h^n|\phi_h^n\rangle$. This underlies the observation reported in [10] which there is misinterpreted as restoration of energy after perturbation.

It is interesting to see, [13], that U_h arrises also from a symmetric Trotter-Suzuki representation of $\exp(hD_{\mathrm{mix}})$: Using the decomposition

$$D_{\mathrm{mix}} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ D^2 & 0 \end{pmatrix} =: A + B \tag{32}$$

we get operators for which the exponential series consists of only two terms and we easily verify

$$U_h = \exp\left(\frac{h}{2}A\right)\exp(hB)\exp\left(\frac{h}{2}A\right)\,, \tag{33}$$

which is exactly the decomposition (27).

2.1 Explicit representation of the n-th iteration of the integrator

Since U_h^n in (29) is the n-th power of a linear map it can be computed in principle by diagonalization. This would require computation of the eigenvectors and eigenvalues of H, which for most systems of practical interest is hardly possible. However, using such a spectral representation of H as a mathematical tool allows us to derive general properties of the iterated integrator which would not easily be derived from an analysis of trajectories as defined in (30). For orientation and — as will turn out — as the main part of the work, we first consider the case that $\mathcal{H}$ is one-dimensional. Then it is no restriction of generality to interpret $\mathcal{H}$ as $\mathbb{C}$, and H as a real number. We then read the second matrix in equation (28) as a real two by two matrix to get a definition of U_h for this concrete case. One computes the n-th power of this matrix by diagonalization:

$$\begin{aligned} U_h^n &= \begin{pmatrix} Q & -Q \\ 1 & 1 \end{pmatrix}\begin{pmatrix} \lambda_1^n & 0 \\ 0 & \lambda_2^n \end{pmatrix}\frac{1}{2}\begin{pmatrix} 1/Q & 1 \\ -1/Q & 1 \end{pmatrix}\,, \quad \text{where} \\ Q &:= \frac{\sqrt{h^2H^2-4}}{2H} \quad \text{and} \\ \lambda_{1,2} &:= 1 - \frac{h^2H^2}{2} \mp \frac{hH}{2}\sqrt{h^2H^2-4}\,. \end{aligned} \tag{34}$$

Obviously $\lambda_1\lambda_2 = 1$. For $|hH| < 2$ we get intermediary complex expressions for a real final result, and also in the case $|hH| > 2$, where everything is real, one can transform the terms such that the dependence on n becomes more transparent. A straightforward

calculation gives

$$
\begin{aligned}
U_h^n &= \begin{pmatrix} \cos(nh\hat{B}) & \frac{\hat{A}}{H}\sin(nh\hat{B}) \\ -\frac{H}{\hat{A}}\sin(nh\hat{B}) & \cos(nh\hat{B}) \end{pmatrix}, \quad \lambda_{1,2} = \exp\left(\mp \mathrm{i}\, h\hat{B}\right), \quad \text{where} \\
\hat{A} &:= \sqrt{1-\frac{h^2}{4}H^2}\,, \\
\hat{B} &:= \frac{2}{h}\arctan\frac{hH}{2\hat{A}} = H(1+\frac{1}{24}h^2H^2+\frac{3}{640}h^4H^4)+O(h^6)
\end{aligned}
\tag{35}
$$

in the first case, and

$$
\begin{aligned}
U_h^n &= (-1)^n \begin{pmatrix} \cosh\left(nh\tilde{B}\right) & \frac{\tilde{A}}{H}\sinh\left(nh\tilde{B}\right) \\ \frac{H}{\tilde{A}}\sinh\left(nh\tilde{B}\right) & \cosh\left(nh\tilde{B}\right) \end{pmatrix}, \quad \lambda_{1,2} = -\exp\left(\pm h\tilde{B}\right), \quad \text{where} \\
\tilde{A} &:= \sqrt{\frac{h^2}{4}H^2-1}\,, \\
\tilde{B} &:= \frac{1}{h}\log(hH\tilde{A}+\frac{h^2H^2}{2}-1)\,,
\end{aligned}
\tag{36}
$$

in the second case, and finally

$$
U_h^n = (-1)^n \begin{pmatrix} 1 & 0 \\ nhH^2 & 1 \end{pmatrix}, \quad \lambda_{1,2} = -1\,, \tag{37}
$$

for the degenerate case $|hH| = 2$. In the first case, there is a bound for $\| U_h^n \|$ which is independent of n, whereas in the second case $\| U_h^n \|$ grows exponentially with n. It is natural to refer to these three cases as *stable*, *unstable*, and *indifferent*.

Let us now return to the general case in which $\mathcal{H}$ is d-dimensional. To reduce this case to (35), (36), (37) we choose a spectral decomposition $(e_i)_{i=1}^d$, $(\varepsilon_i)_{i=1}^d$ of H where the e_i are the eigenvectors in $\mathcal{H}$ and ε_i the eigenvalues, and the indexing is done such that $i < j \Rightarrow |\varepsilon_i| \leq |\varepsilon_j|$. Then $|\varepsilon_d| = \| H \|$. For all $i \in I := \{1,\ldots,d\}$ the projector $\mathbf{P}_i := |e_i\rangle\langle e_i|$ commutes with H and the projector $P_i := \mathbf{P}_i \oplus \mathbf{P}_i$ commutes with U_h, and, hence, with U_h^n. Therefore, the 2-dimensional subspace $\mathcal{H}_i := P_i(\mathcal{H}_d)$ is invariant under U_h. The restriction of U_h^n to $\mathcal{H}_i$, when written as a complex two by two matrix, is given by (34) with H replaced by ε_i. The h-dependent partition $I = \hat{I}_h \cup \tilde{I}_h \cup \bar{I}_h$ with

$$
\hat{I}_h := \{i \in I \,:\, |\varepsilon_i h| < 2\}\,, \quad \tilde{I}_h := \{i \in I \,:\, |\varepsilon_i h| > 2\}\,, \quad \bar{I}_h := \{i \in I \,:\, |\varepsilon_i h| = 2\}\,, \tag{38}
$$

decides whether for $i \in I$ this complex two by two matrix equals the matrix in (35), or (36), or (37), again with H replaced by ε_i. The projectors

$$
\hat{\mathbf{P}}_h := \sum_{i\in\hat{I}_h} \mathbf{P}_i\,, \quad \tilde{\mathbf{P}}_h := \sum_{i\in\tilde{I}_h} \mathbf{P}_i\,, \quad \bar{\mathbf{P}}_h := \sum_{i\in\bar{I}_h} \mathbf{P}_i\,, \tag{39}
$$

unveil their origin by satisfying the inequalities

$$
\| hH\hat{\mathbf{P}}_h\psi \| < 2\,\| \hat{\mathbf{P}}_h\psi \|\,, \quad \| hH\tilde{\mathbf{P}}_h\psi \| > 2\,\| \tilde{\mathbf{P}}_h\psi \|\,, \quad \| hH\bar{\mathbf{P}}_h\psi \| = 2\,\| \bar{\mathbf{P}}_h\psi \| \tag{40}
$$

for all $\psi \in \mathcal{H}$. The augmented projectors

$$\hat{P}_h := \hat{\mathbf{P}}_h \oplus \hat{\mathbf{P}}_h \,, \quad \tilde{P}_h := \tilde{\mathbf{P}}_h \oplus \tilde{\mathbf{P}}_h \,, \quad \bar{P}_h := \bar{\mathbf{P}}_h \oplus \bar{\mathbf{P}}_h \,, \tag{41}$$

allow us to decompose the space $\mathcal{H}_d$ into subspaces on which U_h^n is uniform with respect to the property of being stable, unstable, or indifferent. Of course, the projectors in (41) commute with U_h^n and with each other, and add up to the unit-operator. Therefore, the restriction of U_h^n to the invariant subspace $\hat{P}_h(\mathcal{H}_d)$ is the expression for U_h^n as given in (35) with H interpreted again as an operator in $\mathcal{H}$ instead of a real number. Corresponding statements hold for the invariant subspaces $\tilde{P}_h(\mathcal{H}_d)$ and $\bar{P}_h(\mathcal{H}_d)$. We thus have the following *explicit representation* of U_h^n:

$$U_h^n = \hat{U}_h^n \hat{P}_h + \tilde{U}_h^n \tilde{P}_h + \bar{U}_h^n \bar{P}_h \,, \tag{42}$$

where $\hat{U}_h^n$ is the expression as given in (35) for U_h^n with H interpreted an operator in $\mathcal{H}$. In the same manner $\tilde{U}_h^n$ is understood to originate from (36), and $\bar{U}_h^n$ from (37). All functions of H appearing in these expressions are primarily defined via spectral decomposition of H, just as they originated here. They may be defined also by inserting operators into the power series expansions of the corresponding numerical functions.

According to our ordering of the eigenvalues, the set $\hat{I}_h$ grows monotonic to I as $|h|$ tends to zero, and $\tilde{I}_h \cup \bar{I}_h$ shrinks monotonic to the void set. Whenever

$$|h| \, \| H \| < 2 \tag{43}$$

we have $\hat{I}_h = I$ and thus $\hat{P}_h = 1$. Then only the first term in (42) is present.

We are now interested in the behavior of U_h^n for small h, especially in $\lim_{n\to\infty} U_{t/n}^n$ and thus rightfully assume (43). Expansions in powers of h of the quantities $\hat{A}$ and $\hat{B}$ unveils the behavior of of U_h^n near the limit. $\hat{B}$ gives rise to the expansion

$$\hat{B} = H\,(1 + \frac{1}{24}h^2H^2 + \frac{3}{640}h^4H^4 + \frac{5}{7168}h^6H^6 + \frac{35}{294912}h^8H^8 + \dots\ ) =: \hat{H}(h) \,, \tag{44}$$

and the quantities $\hat{A}$ and $\frac{1}{\hat{A}}$ expand as follows:

$$\begin{aligned} \hat{A} &= 1 - \frac{1}{8}h^2H^2 - \frac{1}{128}h^4H^4 - \dots \ &=: \hat{A}_1(h) \,, \\ \frac{1}{\hat{A}} &= 1 + \frac{1}{8}h^2H^2 + \frac{3}{128}h^4H^4 + \dots \ &=: \hat{A}_2(h) \,. \end{aligned} \tag{45}$$

Equation (42) then implies

$$U_h^n = \begin{pmatrix} \cos(nh\hat{H}(h)) & \frac{1}{H}\hat{A}_1(h)\,\sin(nh\hat{H}(h)) \\ -H\hat{A}_2(h)\,\sin(nh\hat{H}(h)) & \cos(nh\hat{H}(h)) \end{pmatrix} . \tag{46}$$

Since $\hat{H}(0) = H$, $\hat{A}_1(0) = \hat{A}_2(0) = 1$, we have

$$\lim_{n\to\infty} U_{t/n}^n = \begin{pmatrix} \cos tH & \frac{1}{H}\sin tH \\ -H\sin tH & \cos tH \end{pmatrix} =: U_t^\infty = \exp\left(t\,D_{\mathrm{mix}}\right) \,, \tag{47}$$

and after some calculation

$$\lim_{n\to\infty}\left(U_{t/n}^{n}-U_{t}^{\infty}\right)n^{2}=-\frac{t^{3}H^{3}}{24}\begin{pmatrix}\sin tH & \frac{1}{H}(3\frac{\sin tH}{tH}-\cos tH)\\ H(3\frac{\sin tH}{tH}+\cos tH) & \sin tH\end{pmatrix}. \tag{48}$$

Applying operator (46) to an initial dynamical state in $\mathcal{H}_0$ and re-building the exponential function from the trigonometric functions gives

$$U_{h}^{n}\begin{pmatrix}\psi\\ -\mathrm{i}H\psi\end{pmatrix}=\begin{pmatrix}\exp\left(-\mathrm{i}nh\hat{H}(h)\right)\psi+\mathrm{i}\hat{A}_{3}(h)\sin(nh\hat{H}(h))\psi\\ -\mathrm{i}H\left(\exp\left(-\mathrm{i}nh\hat{H}(h)\right)-\mathrm{i}\hat{A}_{4}(h)\sin(nh\hat{H}(h))\right)\psi\end{pmatrix}, \tag{49}$$

where

$$\begin{aligned}\hat{A}_{3}(h)&=\frac{1}{8}h^{2}H^{2}+\frac{1}{128}h^{4}H^{4}+\ldots\quad,\\ \hat{A}_{4}(h)&=\frac{1}{8}h^{2}H^{2}+\frac{3}{128}h^{4}H^{4}+\ldots\end{aligned} \tag{50}$$

are the expansions of $1-\hat{A}$ and $\frac{1-\hat{A}}{\hat{A}}$.

To understand the effect of replacing the exact dynamics by (49), we assume that ψ is an eigenvector of H with eigenvalue ε, and that the step size h satisfies $h^2\varepsilon^2<4$. Further, we consider only the state component and not the velocity. The main effect is that the dynamical phase factor $\exp(-\mathrm{i}t\varepsilon)$, $t:=nh$, gets replaced by $\exp\left(-\mathrm{i}t\varepsilon(1+\frac{1}{24}h^2\varepsilon^2)\right)$ and that the term $-\mathrm{i}\frac{1}{8}h^2\varepsilon^2\sin(t\varepsilon(1+\frac{1}{24}h^2\varepsilon^2))\psi$ gets added to the state. If $|h|$ is close to the stability limit $\frac{2}{|\varepsilon|}$ then these modifications are significant: The amplitude-changing additive term has 50 percent of the amplitude of the main term, and the frequency of the main term is shifted by 16 percent. However, if one reduces h to a tenth of the value given by the stability limit, the amplitude-changing additive term shrinks to 0.5 percent of the main term. The frequency shift is still large enough that the simulated wave runs out of phase by a full period after 600 oscillations.

In a sense, the Hamiltonian H acts as a renormalized Hamiltonian $H(1+\frac{1}{24}h^2H^2)$. Replacing the original Hamiltonian by $H(1-\frac{1}{24}h^2H^2)$ would let the new renormalized Hamiltonian come close to the original H.

In a realistic time-discrete model of a quantum system, space is discretized too and the Hamiltonian (and its eigenvalues) depends on the spatial discretization length. A meaningful assessment of the accuracy with which a discretized system is able to represent a continuous one, needs to take the interplay of both discretizations into account. As a rule, one may trust all numerical or graphical results from a simulation if a significant and consistent increase of the resolution does not change the results within the accuracy requirements of the study. For a non-relativistic system like the one in [11], going to half the lattice spacing increases the norm of the Hamiltonian by a factor of 4 and thus asks for changing the time step to a quarter of the original one. The computational burden thus increases by a factor of 16. It would increase by a factor of 32 for a system in three spatial dimensions. This shows that one may be forced to consider less drastic increments of the spatial resolution for testing.

2.2 Semi-conservation of the norm of the initial state

Let us consider the sequence of states in equation (30). For the exact version $\exp(nhD_{\mathrm{mix}})(\psi, D\psi)$ of (ψ_h^n, ϕ_h^n) one would have exact unitarity and exact energy conservation so that the difference quantities

$$\nu(\psi,n,h) := \langle \psi_h^n | \psi_h^n \rangle - \langle \psi | \psi \rangle \,, \quad \varepsilon(\psi,n,h) := \langle \psi_h^n | \phi_h^n \rangle - \langle \psi | \phi \rangle \tag{51}$$

relative to the initial state would vanish for all $n \in \mathbb{N}$. Therefore, these quantities are expected to remain small for trajectories with properly chosen time step h.

The representation (42) gives explicit expressions for the quantities in equation (51). To derive these, we decompose ψ by means of projectors (39):

$$\psi = \hat{\mathbf{P}}_h \psi + \tilde{\mathbf{P}}_h \psi + \bar{\mathbf{P}}_h \psi =: \hat{\psi} + \tilde{\psi} + \bar{\psi} \,. \tag{52}$$

Since the projectors (39) project on mutually orthogonal subspaces, we have

$$\nu(\psi,n,h) = \nu(\hat{\psi},n,h) + \nu(\tilde{\psi},n,h) + \nu(\bar{\psi},n,h) \tag{53}$$

and

$$\varepsilon(\psi,n,h) = \varepsilon(\hat{\psi},n,h) + \varepsilon(\tilde{\psi},n,h) + \varepsilon(\bar{\psi},n,h) \,. \tag{54}$$

From (35) we have

$$\begin{aligned} \nu(\hat{\psi},n,h) &= -\frac{h^2}{4} \, \| H \sin(nh\hat{B}) \, \hat{\psi} \|^2 \,, \\ \varepsilon(\hat{\psi},n,h) &= -\frac{h^2}{8} \langle \hat{\psi} | \, \frac{H^3}{\hat{A}} \sin(2nh\hat{B}) \, \hat{\psi} \rangle \,, \end{aligned} \tag{55}$$

and from (36)

$$\begin{aligned} \nu(\tilde{\psi},n,h) &= \frac{h^2}{4} \, \| H \sinh\left(nh\tilde{B}\right) \, \tilde{\psi} \|^2 \,, \\ \varepsilon(\tilde{\psi},n,h) &= \frac{h^2}{8} \langle \tilde{\psi} | \, \frac{H^3}{\tilde{A}} \sinh\left(2nh\tilde{B}\right) \, \tilde{\psi} \rangle \,, \end{aligned} \tag{56}$$

and, finally, from (37)

$$\begin{aligned} \nu(\bar{\psi},n,h) &= 0 \,, \\ \varepsilon(\bar{\psi},n,h) &= 4 \, \frac{n}{h} \langle \bar{\psi} | \, \bar{\psi} \rangle \,. \end{aligned} \tag{57}$$

Let us consider ε. These equations say that it is real in all cases. This is what we already know from the symplecticity of the algorithm, see (31): since the imaginary part of (ψ_h^n, ϕ_h^n) is independent of n, the imaginary part of the difference function ε is 0. The quantity ν is real by definition and ν and ε are related for the exact solution by (23) and a similar equation can be derived here. Actually, (35) and (36) imply

$$nh\,\varepsilon(\psi,n,h) = \left(\frac{h}{2} \frac{\mathrm{d}}{\mathrm{d}h} - 1 \right) \nu(\psi,n,h) \tag{58}$$

for all h such that $\bar{P}_h\psi = 0$. We will see later how this is related to (23).

Now we consider ν. The first equation in (56) says that $\langle \psi_h^n \,|\, \psi_h^n \rangle$ grows exponentially with n if $\tilde{\mathbf{P}}_h\psi$ does not vanish. This is very likely to be seen in any simulation run in which the step duration h was chosen at random. The present theory assures: Reduction of $|h|$ will finally achieve $\hat{\mathbf{P}}_h\psi = \psi$ and thus $\tilde{\mathbf{P}}_h\psi = 0$ and $\bar{\mathbf{P}}_h\psi = 0$. Then the equations (55) are active with $\hat{\psi} = \psi$. This then implies that $\nu(\psi, n, h)$ will never become positive, i.e. the norm of the evolving state will never exceed the norm of the initial state. Even states with extreme spikes and jumps are no exception to this rule. However, exponential growth will let even tiny components $\tilde{\mathbf{P}}_h\psi$ become dominant and explode . The only reliable way to prevent such components from being present in the initial state of a computational model employing finite precision floating point arithmetics, is to set h such that the state-independent criterion (43) is satisfied. Therefore, in order to cover a time span T we need at least $\frac{T\|H\|}{2}$ steps, which means $T\,\|\,H\,\|$ applications of the Hamilton operator to a state. Exactly the same holds for the leap-frog algorithm (2) which seems to have been applied to the Schrödinger equation first in [2]. With about the same number of applications of the Hamilton operator the *Chebyshev method* [3],[9],[12] is capable of computing the state at time T with a precision which is only limited by rounding errors. This precisely known final state implies no knowledge concerning the trajectory which connects the final state with the initial state. Further, the method is not applicable to time-dependent Hamilton operators — at least not as it stands. For unitary integration methods, e.g. the uncondtionally stable methods [7], the step size is not determined by $\|\,H\,\|$ but by the spectral content of the inital state. Employing the spectral decomposition $(e_i)_{i=1}^d$, $(\varepsilon_i)_{i=1}^d$ of H from (38) we write the inital state as $\psi = \sum_{i=1}^d c_i\, e_i$. Then $|e_l|$, where l is the largest index for which c_l is not neglectably small, sets the time step as $h := \frac{2\pi}{n|e_l|}$, where n is a number which is reasonable as a number of sampling points for a full period, e. g. $n = 16$. For lattice models with many lattice points and initial states that vary slowly from point to point, this step size may be considerably larger than the one which is determined by the maximum energy states of the system.

Finally, we analyze how the functions ν and ε behave in the limit $h \to 0$. For the scaled quantities

$$\nu_s(\psi, n, h) := \frac{\nu(\psi, n, h)}{h^2}\,, \quad \varepsilon_s(\psi, n, h) := \frac{\varepsilon(\psi, n, h)}{h^2} \tag{59}$$

the expansion (44) shows

$$\begin{aligned} \nu_s(\hat{\psi}, n, h) &= -\frac{1}{4}\,\|\,H \sin(nh\hat{H}(h))\,\hat{\psi}\,\|^2 \xrightarrow{h\to 0} -\frac{1}{4}\,\|\,H \sin(nhH)\,\hat{\psi}\,\|^2 =: \tilde{\nu}(\hat{\psi}, nh)\,, \\ \varepsilon_s(\hat{\psi}, n, h) &= -\frac{1}{8}\langle\,\hat{\psi}\,|\,H^3 \sin(2nh\hat{H}(h))\,\hat{\psi}\,\rangle \xrightarrow{h\to 0} -\frac{1}{8}\langle\,\hat{\psi}\,|\,H^3 \sin(2nhH)\,\hat{\psi}\,\rangle =: \tilde{\varepsilon}(\hat{\psi}, nh)\,. \end{aligned} \tag{60}$$

As a result of this, simulation runs of a system for different values of the time step give nearly identical curves for the quantities ν_s and ε_s if represented as functions of time $t = nh$ and not simply as as a function of the step number n. For the scaling limits $\tilde{\nu}$ and $\tilde{\varepsilon}$ one verifies directly $\frac{\mathrm{d}}{\mathrm{d}t}\tilde{\nu}(\psi, t) = 2\tilde{\varepsilon}(\psi, t)$ which can also be derived from the equation (58) for the unscaled quantities. It also agrees with equation (23) for the exact integration. Whilst the scaled versions of ν and ε tend to a finite limit, as $h \to 0$,

the unscaled quantities tend rapidly to 0. Each halving of the time step quarters these quantities. This implies that $\langle \psi_h^n | \psi_h^n \rangle$ remains very close to $\langle \psi | \psi \rangle$, and that the real part of $\langle \psi_h^n | \phi_h^n \rangle$ remains very small.

The behavior of the function $\tilde{\nu}$ becomes transparent by means of the spectral representation of H which was used earlier:

$$\begin{aligned} \tilde{\nu}(\psi,t) &= -\frac{1}{4}\sum_{i=1}^{d} |c_i|^2 \varepsilon_i{}^2 \sin^2(t\varepsilon_i) = -\frac{1}{8}\sum_{i=1}^{d} |c_i|^2 \varepsilon_i{}^2 (1-\cos(2t\varepsilon_i)) \\ &= -\frac{1}{8}\,\|H\psi\|^2 + \frac{1}{8}\sum_{i=1}^{d} |c_i|^2 \varepsilon_i{}^2 \cos(2t\varepsilon_i)\ . \end{aligned} \tag{61}$$

This shows that the function $\tilde{\nu}$, which starts from $\tilde{\nu}(\psi,0) = 0$, drops very fast to a small negative value around which it then oscillates with various frequencies and amplitudes; only if these oscillations conspire in a very specific way the function may come back to zero again. This then means that the norm of state comes exactly back to the initial value. Using the reversibility of the integrator it is easy to construct states which exhibit this property for just one point in time. Such reverted states will, however, exhibit a small component outside $\mathcal{H}_0$.

3 Conclusion

Since the method uses the square of the Hamilton operator it should be particularly useful for relativistic systems. There, the square of the Hamiltonian is always of the form $M^2 + \vec{P}^2$, where M and $\vec{P}$ are the operators of rest mass and three-momentum respectively, and thus may have a simpler structure than the Hamiltonian itself.

Since the method is very simple to code it is well-suited for experimentation. In the application to a Maxwell equation problem in [9] the method reproduced the limit of stability and the accuracy reported there for the Yee method.

The norm of the Hamilton operator should not be very much larger than the highest energies appearing in a spectral decomposition of the states of interest. Otherwise we have a stiff system where the time step of integration is set by an energy scale we are not interested in, but which invades the computation through amplification of numerical noise. For lattice systems as the one in [11] this means that one has to be careful not to use more points than really needed. For the system in [11] there was a beneficial side-effect of this circumstance. The timestep enforced by stability considerations was well suited for rendering the physically interesting features with good accuracy.

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