Exact mapping of Schrödinger equations & Applications

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Contents

1 Hagedorn wavepackets

Consider the time-dependent Schrödinger equation in $\mathbb{R}^d$,

$$i\frac{\partial \psi}{\partial t} = \hat{H}\psi = -\frac{1}{2}\mathrm{Tr}[B : \nabla^2 \psi] + V(x)\psi \tag{1.1}$$

where $B \in \mathbb{R}^{d\times d}$ is a positive definite matrix and $V(x)$ is the potential function in $\mathbb{R}^d$. The first Hagedorn wavepacket are defined by

$$\varphi_0[q,p,Q,P](x) = \pi^{-\frac{d}{4}}(\det Q)^{-\frac{1}{2}} \exp\left(\frac{i}{2}(x-q)^{\mathrm{T}} P Q^{-1}(x-q) + ip^{\mathrm{T}}(x-q)\right) \tag{1.2}$$

with $q, p \in \mathbb{R}^d$ and $Q, P \in \mathbb{C}^{d\times d}$ satisfy the symplecticity relations [1] so that (1.2) is a Gaussian wavepacket. Other wavepackets are defined recursively by

$$\varphi_{k+\langle j\rangle} = \frac{1}{\sqrt{k_j+1}} \hat{A}_j^{\dagger} \varphi_k, \quad j = 1, \cdots, d \tag{1.3}$$

with the ladder operator defined by

$$\hat{A} = -\frac{i}{\sqrt{2}}\Big(P^{\mathrm{T}}(\hat{q}-q) - Q^{\mathrm{T}}(\hat{p}-p)\Big) \tag{1.4}$$

The key properties of the Hagedorn wavepackets are given in the following theorem:

Theorem 1 (Hagedorn) *The Hagedorn wavepackets $\varphi_k = \varphi_k[q,p,Q,P]$ defined by (1.2)(1.3) form a complete L^2-orthonormal set of fucntions. Moreover, if the external potential $V(x)$ is quadratic, let $\big(q(t),p(t),Q(t),P(t)\big)$ be the solution of classical equations of motion*

$$\dot{q} = Bp, \qquad \dot{p} = -\nabla V(q), \qquad \dot{Q} = BP, \qquad \dot{P} = -\nabla^2 V(q)P \tag{1.5}$$

and let

$$S(t) = \int_0^t \left(\frac{1}{2}|p(s)|^2 - V(q(s))\right)\mathrm{d}s \tag{1.6}$$

be the corresponding classical action. Then, for for every multi-index k,

$$\Psi_k(x,t) = e^{iS(t)}\varphi_k[q(t),p(t),Q(t),P(t)](x) \tag{1.7}$$

is a solution of the time-dependent Schrödinger equation (1.1).

It's important to note that although the potential function $V(q)$ is independent of time in the Schrödinger equation (1.1), the solution (1.7) is also valid when V depdends on t. In fact, the definition of the action $S(t)$ is equivalent to the initial value problem

$$\dot{S}(t) = \frac{1}{2}|p(t)|^2 - V(q(t)), \qquad S(0) = 0 \tag{1.8}$$

and the time derivative of $\Psi_k(x,t)$ satisfies

$$\frac{\partial_t \Psi_k(x,t)}{\Psi_k(x,t)} = i\dot{S}(t) + \frac{\partial_q \varphi_k}{\varphi_k}\dot{q}(t) + \frac{\partial_p \varphi_k}{\varphi_k}\dot{p}(t) + \frac{\partial_Q \varphi_k}{\varphi_k}\dot{Q}(t) + \frac{\partial_P \varphi_k}{\varphi_k}\dot{P}(t) \tag{1.9}$$

which is an analytic expression of the parameters $p(t), q(t), P(t), Q(t)$.

Now if the initial value of the Schrödinger equation is

$$\Psi(x,0) = \sum_k c_k \Psi_k(x,0) = e^{iS(0)} \sum_k c_k \varphi_k[q(0),p(0),Q(0),P(0)](x) \tag{1.10}$$

then the solution is given by

$$\Psi(x,t) = \sum_k c_k \Psi_k(x,0) = e^{iS(t)} \sum_k c_k \varphi_k[q(t),p(t),Q(t),P(t)](x) \tag{1.11}$$

and the coefficients $\{c_k\}$ are constant in time.

Comments on the Hagedorn wavepackets:

1. Hagedorn wavepackets write a series of explicit solutions $\{\Psi_k(x,t)\}$ to the Schrödinger equation (1.1), even if the coefficient $B \in \mathbb{R}^{d\times d}$ and the quadratic potential function $V(x)$ in (1.1) depend on time.

2. The basis functions $\{\varphi_k\}$ defined in (1.2) and (1.3) are essentially transformed Hermitian functions. Since $\{\varphi_k\}$ form a complete orthonormal basis of $L^2(\mathbb{R}^d)$, any initial data $\Psi(x,0)$ in $L^2(\mathbb{R}^d)$ can be expanded in the basis. However, in many cases we only consider the initial data in the form of Gaussian wavepackets (1.2).

3. The solution $\Psi_k(x,t)$ is exact only when the potential function $V(x)$ is quadratic. In the general case, the solution may not be analytic.

4. Given the coefficient $B \in \mathbb{R}^{d\times d}$ and potential function $V(x)$, any set of the initial values of the parameters q, p, Q, P yield a valid solution to the Schrödinger equation (1.1). Therefore, $\{\varphi_k(x)\}$ has no connection with the eigenfunctions of $\hat{H}$.

2 Spectral method for Schrödinger equation

2.1 Schrödinger-type ODE system

We aim to solve the time-depdendent Schrödinger equation

$$i\frac{\partial \psi}{\partial t} = \hat{H}\psi \tag{2.1}$$

with the Hamiltonian operator given by

$$\hat{H} = \hat{H}_0 + \hat{H}_p \tag{2.2}$$

Both $\hat{H}_0$ and $\hat{H}_p$ can depend on time. Assume $\hat{H}_0$ is simple enough constitutes the main part of the total Hamiltonian $\hat{H}$, and the solution of the truncated Schrödinger equation

$$i\frac{\partial \psi}{\partial t} = \hat{H}_0\psi \tag{2.3}$$

can be explicitly written as a series of wavefunctions $\{\Psi_k(x,t)\}$. We require $\{\Psi_k(x,t)\}$ to form a complete basis so that any initial data $\Psi(x,0)$ can be expanded in the basis. Typical examples of $\hat{H}_0$ and the corresponding solutions $\Psi_k(x,t)$ include:

1. $\hat{H}_0 = -\frac{1}{2}\Delta$ with periodic boundary conditions in the interval $[a,b]$.

$$E_k = \left(\frac{2k\pi}{b-a}\right)^2, \qquad \phi_k(x) = \exp\left(i2k\pi\cdot\frac{x-a}{b-a}\right), \qquad k\in\mathbb{Z}$$

   The solution is

$$\Psi_k(x,t) = e^{iE_kt}\phi_k(x)$$

2. $\hat{H}_0 = -\frac{1}{2}\Delta + \frac{1}{2}\hat{x}^2$ in the real line. The eigenfunctions ar the Hermite functions[1], i.e.,

$$E_n = n + \frac{1}{2}, \qquad \phi_n(x) = \frac{1}{\sqrt{2^n n!}}\frac{1}{\sqrt[4]{\pi}}e^{-\frac{x^2}{2}}H_n(x), \qquad n = 0,1,2,\cdots$$

[1] See `https://en.wikipedia.org/wiki/Quantum_harmonic_oscillator` for detailed explanation.

where $H_n(x)$ are the Hermite polynomials,

$$H_n(x) = (-1)^n e^{x^2} \frac{\mathrm{d}^n}{\mathrm{d}x^n}\left(e^{-x^2}\right)$$

The solution is

$$\Psi_k(x,t) = e^{iE_k t}\phi_k(x)$$

3. $\hat{H}_0 = -\frac{1}{2}\mathrm{Tr}[B : \nabla^2] + V(x,t)$ and $V(x,t)$ is quadratic for any time t. The basis solution is represented as Hagedorn wavepackets defined in (1.7).

Now we consider the ansatz for the general Schrödinger equation (2.2)

$$\Psi(x,t) = \sum_k c_k(t)\Psi_k(x,t) \tag{2.4}$$

where each $\Psi_k(x,t)$ is the solution of the truncated system (2.3). Then

$$\begin{aligned} i\frac{\partial \Psi}{\partial t} &= i\sum_k \dot{c}_k(t)\Psi_k(x,t) + i\sum c_k \frac{\partial \Psi_k(x,t)}{\partial t} \\ &= i\sum_k \dot{c}_k(t)\Psi_k(x,t) + \hat{H}_0\Psi \end{aligned}$$

which implies

$$i\sum_k \dot{c}_k(t)\Psi_k(x,t) = \hat{H}_p\Psi(x,t) = \sum_l c_l(t)\hat{H}_p\Psi_l(x,t) \tag{2.5}$$

Taking $\Psi_k(x,t)$ as the test fucntion, we obtain

$$i\dot{c}_k(t) = \sum_l f_{kl}c_l(t) \tag{2.6}$$

where

$$f_{kl} := \langle \Psi_k | \hat{H}_p | \Psi_l \rangle = \int_{\mathbb{R}} \overline{\Psi_k(x,t)}\hat{H}_p\Psi_l(x,t)\mathrm{d}x$$

Note that $\hat{H}_p$ is Hermitian implies that the coefficient matrix $\{f_{kl}\}_{N\times N}$ is Hermitian, hence the ODE system (2.6) behaves like a Schrödinger equation.

2.2 Calculation of the coefficient f_{kl}

Now we aim to compute coeffient

$$f_{kl} := \langle \Psi_k | \hat{H}_p | \Psi_l \rangle \tag{2.7}$$

In the simplest case, assume the truncated Hamiltonian $\hat{H}_0$ is the harmonic oscillator, i.e.,

$$\hat{H}_0 = -\frac{1}{2}\Delta + \frac{1}{2}\hat{x}^2 \tag{2.8}$$

and the basis functions are $\Psi_k(x,t) = e^{iE_k t}\phi_k(x)$. Assume $\hat{H}_p = h(\hat{x})$ is a polynomial of $\hat{x}$, then

$$\begin{aligned} f_{kl} &= \langle \Phi_k | \hat{H}_p | \Phi_l \rangle \\ &= \int_{\mathbb{R}} \phi_k(x) h(x) \phi_l(x) \mathrm{d}x \\ &= \frac{1}{\sqrt{2^k k!}} \frac{1}{\sqrt{2^l l!}} \frac{1}{\sqrt{\pi}} \int_{\mathbb{R}} e^{-x^2} H_k(x) H_l(x) h(x) \end{aligned}$$

Suppose $h(x)$ is decomposed as

$$h(x) = \sum_m h_m H_m(x) \tag{2.9}$$

with the coefficients $\{h_m\}$, we have

$$f_{kl} = \frac{1}{\sqrt{2^k k!}} \frac{1}{\sqrt{2^l l!}} \frac{1}{\sqrt{\pi}} \sum_m h_m \int_{\mathbb{R}} e^{-x^2} H_k(x) H_l(x) H_m(x) \mathrm{d}x \tag{2.10}$$

Using the fact that[2]

$$\int_{\mathbb{R}} e^{-x^2} H_k(x) H_l(x) H_m(x) \mathrm{d}x = \frac{2^{\frac{1}{2}(k+l+m)} k!\, l!\, m! \sqrt{\pi}}{\left(\frac{1}{2}(k+l-m)\right)! \left(\frac{1}{2}(-k+l+m)\right)! \left(\frac{1}{2}(k-l+m)\right)!} \tag{2.11}$$

when $k+l \geqslant m$, $k+m \geqslant l$, $l+m \geqslant k$ and $2 \mid k+l+m$, we obtain

$$f_{kl} = \sum_m \frac{2^{\frac{m}{2}} \sqrt{k!\, l!}\, m!}{\left(\frac{1}{2}(k+l-m)\right)! \left(\frac{1}{2}(-k+l+m)\right)! \left(\frac{1}{2}(k-l+m)\right)!} h_m \tag{2.12}$$

Especially, when $\hat{H}_p(x) \equiv 1$, $f_{kl} = \delta_{kl}$. In the numerical tests, we choose

$$h(x) = \frac{1}{16} H_4(x) + \frac{1}{2} H_1(x) = x^4 - 4x^2 + x + \frac{3}{4} \tag{2.13}$$

which implies the coefficient $h_1 = \frac{1}{2}$ and $h_4 = \frac{1}{16}$. Note that the matrix $\{f_{kl}\}$ is real-valued and symmetric.

Stiffness of the ODE system:

The ODE system (2.6) is stiff when the number of basis functions is large. In fact, the expression of f_{kl} (2.12) implies that f_{kl} is extremely large when k, l are big, thus small timesteps are required to integrate the dynamics, unless a strongly stable numerical integrator is employed.

2.3 Time splitting method

We briefly introduce the time splitting method, whose idea to integrate the two dynamics

$$i\frac{\partial \psi}{\partial t} = \hat{H}_0 \psi, \qquad i\frac{\partial \psi}{\partial t} = \hat{H}_p \psi \tag{2.14}$$

[2] `https://functions.wolfram.com/Polynomials/HermiteH/21/ShowAll.html`

respectively. Usually, $\hat{H}_0 = -\frac{1}{2}\Delta$ or $\hat{H}_0 = -\frac{1}{2}\Delta + \frac{1}{2}\omega^2\hat{x}^2$, which corresponds to the Fourier [2] and Hermite [3] spectral methods respectively. In this way, the Schrödinger equation for $\hat{H}_0$ can be solved explicitly using the spectral method, and the equation for $\hat{H}_p$ can be directly solved in the physical space.

It's important to note that there is no stiffness in the time splitting method, and the only technique is the transformation from the physical space to the frequency space.

3 Numerical integrator for Schrödinger-type ODE

3.1 Real-imaginary splitting technique

Consider Schrödinger-like ODE for $\{c_k(t)\}_{k=1}^N$:

$$i\dot{c}_k(t) = \sum_l f_{kl}c_l(t) \tag{3.1}$$

where the coefficient matrix $\{f_{kl}\}$ is complex-valued and Hermitian, i.e.,

$$\mathrm{Re}(f_{kl}) = \mathrm{Re}(f_{lk}), \quad \mathrm{Im}(f_{kl}) = -\mathrm{Im}(f_{lk}) \tag{3.2}$$

This means $\mathcal{R} := \{\mathrm{Re}(f_{kl})\}$ is symmetric while $\mathcal{I} := \{\mathrm{Im}(f_{kl})\}$ is anti-symmetric. Write the coefficient $c_k(t)$ in the real and imaginary parts as

$$c_k(t) = a_k(t) + ib_k(t) \tag{3.3}$$

and we obtain the ODE system for $\{a_k(t)\}$ and $\{b_k(t)\}$:

$$\begin{cases} \dot{a}_k(t) = \sum_l \mathrm{Im}(f_{kl})a_l(t) + \sum_l \mathrm{Re}(f_{kl})b_l(t) \\ \dot{b}_k(t) = -\sum_l \mathrm{Re}(f_{kl})a_l(t) + \sum_l \mathrm{Im}(f_{kl})b_l(t) \end{cases} \tag{3.4}$$

or equivalently in the matrix form

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} \mathcal{I} & \mathcal{R} \\ -\mathcal{R} & \mathcal{I} \end{bmatrix}\begin{bmatrix} a \\ b \end{bmatrix} \tag{3.5}$$

which is the Hamiltonian dynamics for

$$H(a,b) = \frac{1}{2}(a^{\mathrm{T}}\mathcal{R}a + b^{\mathrm{T}}\mathcal{R}b) + b^{\mathrm{T}}\mathcal{I}a \tag{3.6}$$

The Hamiltonian dynamics (3.4) satisfies the following conservation laws.

Mass conservation The total mass

$$M(t) := \sum_k |c_k(t)|^2 = \sum_k |a_k(t)|^2 + \sum_k |b_k(t)|^2 \tag{3.7}$$

is conserved along the dynamics. This is because

$$\dot{M}(t) = 2(a^{\mathrm{T}}\dot{a} + b^{\mathrm{T}}\dot{b}) = 2\big(a^{\mathrm{T}}\mathcal{I}a + a^{\mathrm{T}}\mathcal{R}b\big) + 2\big(-b^{\mathrm{T}}\mathcal{R}a + b^{\mathrm{T}}\mathcal{I}b\big) = 0 \tag{3.8}$$

Here we use the fact that

$$\mathcal{R} \text{ is symmetric} \Longrightarrow a^{\mathrm{T}}\mathcal{R}b = b^{\mathrm{T}}\mathcal{R}a$$
$$\mathcal{I} \text{ is anti-symmetric} \Longrightarrow a^{\mathrm{T}}\mathcal{I}a = b^{\mathrm{T}}\mathcal{I}b = 0$$

Energy conservation When $\{f_{kl}\}$ is a constant matrix, the Hamiltonian $H(a, b)$ is conserved along the dynamics. However, this may not be true when $\{f_{kl}\}$ depends on time. In the following we discuss various numerical integrators for the ODE system (3.5).

3.2 Runge-Kutta method

The Runge-Kutta method is the most widely-used integrator in numerical integration. The ODE system (3.5) can be rewritten as the linear system

$$\frac{\mathrm{d}z}{\mathrm{d}t} = Bz \tag{3.9}$$

and the 4th order Runge-Kutta method in a timestep is given by

$$\begin{aligned}
K_1 &= Bz \\
K_2 &= B\Big(z + \frac{K_1}{2}\Delta t\Big) \\
K_3 &= B\Big(z + \frac{K_2}{2}\Delta t\Big) \\
K_4 &= B(z + K_3\Delta t) \\
z &= z + \frac{K_1 + 2K_2 + 2K_3 + K_4}{6}\Delta t
\end{aligned}$$

The Runge-Kutta method has 4th order of accuracy, and the symplectic structure is not guaranteed.

3.3 Symplectic integrator for non-separable Hamiltonian system

Since (3.5) is a Hamiltonian dynamics, it's natural to design a symplectic integrator to expect satisfactory long time performance. The explicit symplectic integrator for separable Hamilonians has been extensively studied, but this is not the case for non-separable Hamiltonians, for example, $H(a, b)$ defined in (3.6). When the imaginary part $\mathcal{I} \in \mathbb{R}^{N\times N}$ is nonzero, the Hamiltonian $H(a, b)$ becomes non-sparable.

We employ the numerical integrator introduced in [4] by Molei Tao and introduce the augmented Hamiltonian

$$\bar{H}(a, b, a', b') = H(a, b') + H(a', b) + \frac{\omega}{2}(|a - a'|^2 + |b - b'|^2) \tag{3.10}$$

where $\omega > 0$ is a fixed constant. The Hamiltonian dynamics corresponding to $\bar{H}$ is

$$\begin{cases} \dot{a} = \partial_b H(a', b) + \omega(b - b') \\ \dot{b} = -\partial_a H(a, b') - \omega(a - a') \\ \dot{a}' = \partial_b H(a, b') + \omega(b' - b) \\ \dot{b}' = -\partial_a H(a', b) - \omega(a - a') \end{cases} \tag{3.11}$$

The numerical integrator can be constructed in a splitting scheme. In a timestep, denote the numerical integrators by

$$\phi^{\Delta t}_{a,b'} : \begin{bmatrix} a \\ b \\ a' \\ b' \end{bmatrix} \mapsto \begin{bmatrix} a + \partial_b H(a', b)\Delta t \\ b \\ a' \\ b' - \partial_a H(a', b)\Delta t \end{bmatrix} = \begin{bmatrix} a + (\mathcal{I}a' + \mathcal{R}b)\Delta t \\ b \\ a' \\ b' + (-\mathcal{R}a' + \mathcal{I}b)\Delta t \end{bmatrix}$$

$$\phi^{\Delta t}_{a',b} : \begin{bmatrix} a \\ b \\ a' \\ b' \end{bmatrix} \mapsto \begin{bmatrix} a \\ b - \partial_a H(a, b')\Delta t \\ a' + \partial_b H(a, b')\Delta t \\ b' \end{bmatrix} = \begin{bmatrix} a \\ b + (-\mathcal{R}a + \mathcal{I}b')\Delta t \\ a' + (\mathcal{I}a + \mathcal{R}b')\Delta t \\ b' \end{bmatrix}$$

$$\phi^{\Delta t}_{\omega} : \begin{bmatrix} a \\ b \\ a' \\ b' \end{bmatrix} \mapsto \frac{1}{2} \begin{bmatrix} \begin{pmatrix} a + a' \\ b + b' \end{pmatrix} + R(\Delta t) \begin{pmatrix} a - a' \\ b - b' \end{pmatrix} \\ \begin{pmatrix} a + a' \\ b + b' \end{pmatrix} - R(\Delta t) \begin{pmatrix} a - a' \\ b - b' \end{pmatrix} \end{bmatrix}$$

where

$$R(\Delta t) = \begin{bmatrix} \cos(2\omega\Delta t)I & \sin(2\omega\Delta t)I \\ -\sin(2\omega\Delta t)I & \cos(2\omega\Delta t)I \end{bmatrix}$$

and the overall 2nd-order integrator is given by

$$\phi^{\Delta t}_2 := \phi^{\Delta t/2}_{a,b'} \circ \phi^{\Delta t/2}_{a',b} \circ \phi^{\Delta t}_{\omega} \circ \phi^{\Delta t/2}_{a',b} \circ \phi^{\Delta t/2}_{a,b'} \tag{3.12}$$

Finally we obtain the symplectic integrator in Δt time:

Algorithm 1: Symplectic integrator for the non-separable Hamiltonian $H(a, b)$

Input: coordinates $a_0, b_0 \in \mathbb{R}^N$ at initial, timestep Δt
Output: coordinates $a_1, b_1 \in \mathbb{R}^N$ after one timestep
Obtain (a_1, b_1) from the numerical flow $\phi^{\Delta t}_2$:

$$\begin{bmatrix} a_1 \\ b_1 \\ \sim \\ \sim \end{bmatrix} = \phi^{\Delta t}_2 \begin{bmatrix} a_0 \\ b_0 \\ a_0 \\ b_0 \end{bmatrix}$$

Since Tao's integrator above is symplectic, we may construct high-order schemes using the Suzuki-Yoshida method [5]. For example, the 4th-order integrator can be constructed from

$$\phi^{\Delta t}_4 = \phi^{\tau_0 \Delta t}_2 \circ \phi^{\tau_1 \Delta t}_2 \circ \phi^{\tau_0 \Delta t}_2 \tag{3.13}$$

where

$$\tau_0 = \frac{1}{2-\kappa}, \qquad \tau_1 = -\frac{\kappa}{2-\kappa}, \qquad \kappa = 2^{\frac{1}{3}} \tag{3.14}$$

Note that $\tau_1 < 0$ in the symplectic integrator, which is similar with the Richardson extrapolation.

3.4 Implicit symplectic integrator

The explicit integrators above are easy to implement, but extremely small timesteps are required if the ODE system is stiff. However, the high frequency parts do not contribute much to the overall wavefunction, thus a highly stable numerical integrator is preferable.

We still consider the ODE system

$$\frac{\mathrm{d}z}{\mathrm{d}t} = Bz \tag{3.15}$$

where the coefficient matrix

$$B = \begin{bmatrix} \mathcal{I} & \mathcal{R} \\ -\mathcal{R} & \mathcal{I} \end{bmatrix} \tag{3.16}$$

is a infinitesimal symplectic matrix [6, 7] hence the ODE system has symplectic structure. The $2m$-order implicit schemes can be given in the following procedure [7]:

$$z_{n+1} = \frac{P_m(\Delta t B)}{P_m(-\Delta t B)} z_n \tag{3.17}$$

where the polynomials P_m are given by

$$\begin{aligned} P_0(\lambda) &= 1 \\ P_1(\lambda) &= 2 + \lambda \\ P_2(\lambda) &= 12 + 6\lambda + \lambda^2 \end{aligned}$$

In particular, the 2nd-order scheme is given by

$$\Big(I - \frac{1}{2}\Delta t B\Big) z_{n+1} = \Big(I + \frac{1}{2}\Delta t B\Big) z_n \tag{3.18}$$

and the 4th-order scheme is given by

$$\Big(I - \frac{1}{2}\Delta t B + \frac{1}{12}\Delta t^2 B^2\Big) z_{n+1} = \Big(I + \frac{1}{2}\Delta t B + \frac{1}{12}\Delta t^2 B^2\Big) z_n \tag{3.19}$$

When $\mathcal{R}$ is symmetric and $\mathcal{I}$ is anti-symmetric, all the eigenvalues of B are pure imaginary. In fact, assume $x, y \in \mathbb{C}^N$[3] and $\lambda \in \mathbb{C}$ satisfying the eigenvalue problem

$$\begin{bmatrix} \mathcal{I} & \mathcal{R} \\ -\mathcal{R} & \mathcal{I} \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \lambda \begin{bmatrix} x \\ y \end{bmatrix} \tag{3.20}$$

then

$$\mathcal{I}x + \mathcal{R}y = \lambda x, \qquad -\mathcal{R}x + \mathcal{I}y = \lambda y \tag{3.21}$$

[3] We use $x, y \in \mathbb{C}^N$ rather than $a, b \in \mathbb{R}^N$ since a, b are real vectors.

hence

$$\begin{aligned}\lambda(|x|^2+|y|^2) &= x^*(\mathcal{I}x+\mathcal{R}y)+y^*(-\mathcal{R}x+\mathcal{I}y)\\ &= x^*\mathcal{R}y-y^*\mathcal{R}x\\ &= 2\,\mathrm{Im}(x^*\mathcal{R}y)\end{aligned}$$

which implies λ must be a pure imaginary number. Therefore, the implicit schemes above are unconditionally stable. Also, these implicit methods exactly preserve the mass and energy.

3.5 Tests for the numerical integrator

For the Hamiltonian

$$H(a,b)=\frac{1}{2}(a^{\mathrm{T}}\mathcal{R}a+b^{\mathrm{T}}\mathcal{R}b)+b^{\mathrm{T}}\mathcal{I}a$$

and the corresponding Hamiltonian dynamics

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{bmatrix}a\\b\end{bmatrix}=\begin{bmatrix}\mathcal{I}&\mathcal{R}\\-\mathcal{R}&\mathcal{I}\end{bmatrix}\begin{bmatrix}a\\b\end{bmatrix}$$

we test the performance of various numerical integrators including the Runge-Kutta method, explicit and implicit symplectic integrators. Fixing $N=6$, the data of the symmetric $\mathcal{R}$ and the anti-symmetric are given by

$$\mathcal{R}=\begin{bmatrix}1.0753&1.4003&-1.5334&2.2712&0.8077&-0.4193\\1.4003&0.6852&3.5153&4.1866&-0.3152&1.8879\\-1.5334&3.5153&1.4295&0.4665&0.6027&0.4208\\2.2712&4.1866&0.4665&-2.4150&0.4138&0.8207\\0.8077&-0.3152&0.6027&0.4138&0.5877&-3.7316\\-0.4193&1.8879&0.4208&0.8207&-3.7316&2.8768\end{bmatrix} \tag{3.22}$$

$$\mathcal{I}=\begin{bmatrix}0&1.0741&-0.2770&1.7047&-0.9868&-1.2501\\-1.0741&0&1.9742&1.56270.1974&-1.3700&\\0.2770&-1.9742&0&-0.8470&1.7666&0.0519\\-1.7047&-1.5627&0.8470&0&1.3262&1.2331\\0.9868&-0.1974&-1.7666&-1.3262&0&-0.7015\\1.2501&1.3700&-0.0519&-1.2331&0.7015&0\end{bmatrix} \tag{3.23}$$

and the initial values are

$$a_0=\begin{bmatrix}-0.7697\\3.5544\\-3.0594\\-5.6091\\-5.6895\\1.9528\end{bmatrix},\qquad b_0=\begin{bmatrix}-0.7095\\-0.7842\\5.6772\\1.1663\\0.7912\\6.3508\end{bmatrix} \tag{3.24}$$

The numerical performance of the method will be measured in two ways:

1. Energy and mass conservation property.
2. l^2 error at a given simulation time.

For $T = 10^3$, we record the mass and the energy along the simulation for various methods. The timestep is fixed at $\Delta t = 10^{-1}$. The constant ω in the symplectic method is set at 1.

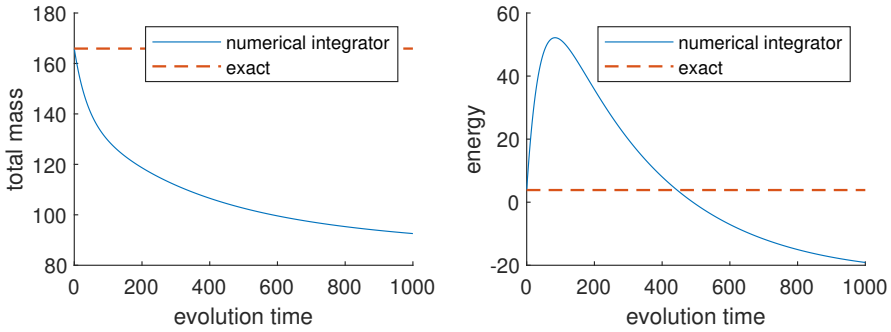

Figure 1: Mass and energy conservation for the 4th-order Runge-Kutta method. Deviation of the mass and energy is 15.11 and 22.96 respectively.

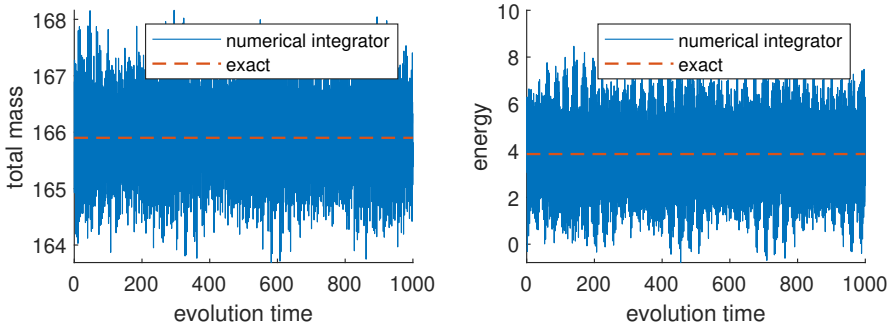

Figure 2: Mass and energy conservation for the 4th-order Runge-Kutta method. Deviation of the mass and energy is 0.64 and 1.39 respectively.

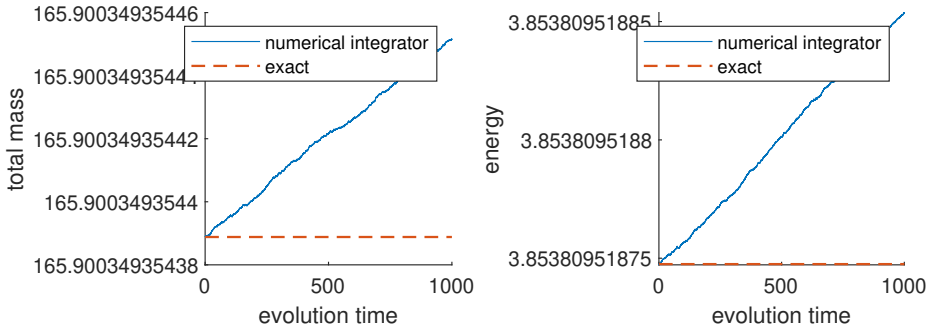

Figure 3: Mass and energy conservation for the 4th-order implicit method. Deviation of the mass and energy is 1.84×10^{-11} and 3.17×10^{-11} respectively.

Next we compute the l^2-error of different methods. At given time $T = 10^3$, the l^2 error of the computed (a, b) is recorded. The reference solution is computed by the 4th-order implicit scheme with $\Delta t = 10^{-4}$.

References

[1] Caroline Lasser and Christian Lubich. Computing quantum dynamics in the semiclassical regime. *Acta Numerica*, 29:229–401, 2020.

[2] Weizhu Bao, Shi Jin, and Peter A Markowich. On time-splitting spectral approximations for the schrödinger equation in the semiclassical regime. *Journal of Computational Physics*, 175(2):487–524, 2002.

[3] M. Thalhammer, M. Caliari, and C. Neuhauser. High-order time-splitting hermite and fourier spectral methods. *Journal of Computational Physics*, 228(3):822–832, 2009.

[4] Molei Tao. Explicit symplectic approximation of nonseparable hamiltonians: Algorithm and long time performance. *Physical Review E*, 94(4):043303, 2016.

[5] Ben Leimkuhler and Charles Matthews. *Molecular Dynamics.* Springer, 2016.

[6] Kang Feng, Hua-mo Wu, and Meng-Zhao Qin. Symplectic difference schemes for linear hamiltonian canonical systems. *Journal of Computational Mathematics*, pages 371–380, 1990.

[7] Pingwen Zhang and Tiejun Li. *Numerical Analysis.* Peking University, 2007.