1 Hamiltonian structure

Consider the scaled Schrödinger equation

$$\dot{\psi} = -iH(t)\psi, \quad \psi(0) = \psi_0, \quad H(t) = H_s + f(t)a + \bar{f}(t)a^\dagger. \tag{1}$$

Here, $\psi \in \mathbb{C}^N$ and $H_s = H_s^\dagger$ is the system Hamiltonian matrix, which we assume to be Hermitian, real-valued, and independent of time. The lowering and raising matrices are denoted a and $a^\dagger$, respectively. These matrices satisfy

$$a = \begin{bmatrix} 0 & 1 & & & & \\ & 0 & \sqrt{2} & & & \\ & & 0 & \sqrt{3} & & \\ & & & 0 & \sqrt{4} & \\ & & & & \ddots & \ddots \end{bmatrix}, \quad a^\dagger = \begin{bmatrix} 0 & & & & & \\ 1 & 0 & & & & \\ & \sqrt{2} & 0 & & & \\ & & \sqrt{3} & 0 & & \\ & & & \ddots & \ddots & \end{bmatrix} \tag{2}$$

The time-dependent control terms in (1) can be written

$$f(t)a + \bar{f}(t)a^\dagger = f_r(t)(a + a^\dagger) + if_i(t)(a - a^\dagger), \quad f_r = \operatorname{Re} f, \quad f_i = \operatorname{Im} f,$$

where $i = \sqrt{-1}$ is the imaginary unit. We conclude that the control terms are Hermitian and $H(t) = H^\dagger(t)$.

To utilize efficient numerical ODE solvers it is desirable to derive a real-valued equivalent of (1). Let the functions $u(t)$ and $v(t) \in \mathbb{R} \to \mathbb{R}^N$ be defined by

$$\psi(t) = u(t) - iv(t)$$

and decompose the total Hamiltonian matrix into $H(t) = K(t) + iS(t)$, where the real-valued matrices K and S hold the symmeric and skew-symmetric parts of H: $K^\dagger = K$ and $S^\dagger = -S$. We have,

$$\begin{aligned} H\psi &= (K + iS)(u - iv) = (Ku + Sv) + i(Su - Kv), \\ -iH\psi &= -i(Ku + Sv) + (Su - Kv). \end{aligned}$$

Therefore, a real-valued equivalent of the system (1) is

$$\begin{bmatrix} \dot{u} \\ \dot{v} \end{bmatrix} = \begin{bmatrix} S(t) & -K(t) \\ K(t) & S(t) \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix}. \tag{3}$$

We define the time-dependent Hamiltonian function to be

$$\kappa(u, v, t) = u^T S(t) v + \frac{1}{2} u^T K(t) u + \frac{1}{2} v^T K(t) v. \tag{4}$$

We have

$$\frac{\partial \kappa}{\partial u_q} = \frac{\partial}{\partial u_q} \sum_{j,k} (u_j S_{j,k} v_k + 0.5 u_j K_{j,k} u_k) = \sum_k (S_{q,k} v_k + 0.5 K_{q,k} u_k) + 0.5 \sum_j u_j K_{j,q}.$$

Because $K^T = K$,

$$\nabla_u \kappa = Sv + Ku.$$

In a similar way,

$$\nabla_v \kappa = S^T u + Kv = -Su + Kv.$$

Therefore, (3) has the Hamiltonian structure

$$\begin{bmatrix} \dot{u} \\ \dot{v} \end{bmatrix} = \begin{bmatrix} -\nabla_v \kappa(u,v,t) \\ \nabla_u \kappa(u,v,t) \end{bmatrix} = \begin{bmatrix} Su - Kv \\ Ku + Sv \end{bmatrix} \tag{5}$$

Because $v^T S^T u = u^T S v$, the Hamiltonian function (4) can be written

$$\kappa(u,v,t) = \frac{1}{2} \begin{bmatrix} u \\ v \end{bmatrix}^T \begin{bmatrix} K(t) & S(t) \\ S^T(t) & K(t) \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix}. \tag{6}$$

We conclude that the Hamiltonian function is non-separable due to the skew-symmetric term $S(t) = f_i(t)(a - a^\dagger)$ in the original Hamiltonian matrix.

1.1 Autonomous Hamiltonian form

A standard approach for transforming a non-autonomous Hamiltonian system into autonomous form is as follows. First introduce the scalar dependent variable $\tau(t) = t$ which satisfies the trivial equation

$$\dot{\tau} = 1, \quad \tau(0) = 0. \tag{7}$$

Hence, $\kappa(u,v,t) = \kappa(u,v,\tau)$. Then introduce a scalar variable $e(t)$ and let it satisfy

$$\dot{e} = -\kappa_t(u,v,t), \quad e(0) = -\kappa(u_0, v_0, 0). \tag{8}$$

where $u_0 = u(0)$ and $v_0 = v(0)$ are the initial data for (5). Next, define the generalized momentum and position variables

$$p = \begin{bmatrix} u \\ e \end{bmatrix}, \quad q = \begin{bmatrix} v \\ \tau \end{bmatrix},$$

and define the extended Hamiltonian function by

$$\tilde{\kappa}(p,q) = \kappa(u,v,\tau) + e.$$

We note that

$$\nabla_q \tilde{\kappa} = \begin{bmatrix} \nabla_v \kappa \\ \kappa_\tau \end{bmatrix}, \quad \nabla_p \tilde{\kappa} = \begin{bmatrix} \nabla_u \kappa \\ 1 \end{bmatrix}.$$

From (5)-(8), the generalized variables satisfy the differential equation

$$\begin{bmatrix} \dot{p} \\ \dot{q} \end{bmatrix} = \begin{bmatrix} \dot{u} \\ \dot{e} \\ \dot{v} \\ \dot{\tau} \end{bmatrix} = \begin{bmatrix} -\nabla_v \kappa(u,v,\tau) \\ -\kappa_\tau(u,v,\tau) \\ \nabla_u \kappa(u,v,\tau) \\ 1 \end{bmatrix} = \begin{bmatrix} -\nabla_q \tilde{\kappa}(p,q) \\ \nabla_p \kappa(p,q) \end{bmatrix}, \tag{9}$$

which is an autonomous Hamiltonian system. By setting $t = \tau$ in (6) and differentiating,

$$\kappa_\tau(u,v,\tau) = \frac{1}{2}\left(u^T K'(\tau)u + u^T S'(\tau)v + v^T S'^T(\tau)u + v^T K'(\tau)v\right). \tag{10}$$

1.2 ρ-reversibility

Let $\rho(y)$ be the linear invertible transformation

$$\rho(y) = \begin{bmatrix} I & 0 \\ 0 & -I \end{bmatrix} \begin{bmatrix} p \\ q \end{bmatrix} = \begin{bmatrix} p \\ -q \end{bmatrix}, \quad y = \begin{bmatrix} p \\ q \end{bmatrix}.$$

We write the autonomous Hamiltonian system (9) as

$$\dot{y} = f(y), \quad f(y) = \begin{bmatrix} -\tilde{\kappa}_q \\ \tilde{\kappa}_p \end{bmatrix}.$$

The differential equation $\dot{y} = f(y)$ and the vector field $f(y)$ are called ρ-reversible if

$$\rho(f(y)) = -f(\rho(y)). \tag{11}$$

We have $\rho(y) = (u, e, -v, -\tau)^T$, so the components of the vector field $f(y)$ and $f(\rho(y))$ are

$$f(y) = \begin{bmatrix} S(\tau)u - K(\tau)v \\ -\kappa_\tau(u,v,\tau) \\ K(\tau)u + S(\tau)v \\ 1 \end{bmatrix}, \quad f(\rho(y)) = \begin{bmatrix} S(-\tau)u + K(-\tau)v \\ -\kappa_\tau(u,-v,-\tau) \\ K(-\tau)u - S(-\tau)v \\ 1 \end{bmatrix}.$$

We also have

$$\rho(f(y)) = \begin{bmatrix} S(\tau)u - K(\tau)v \\ -\kappa_\tau(u,v,\tau) \\ -K(\tau)u - S(\tau)v \\ -1 \end{bmatrix}.$$

Thus the conditions for ρ-reversibility (11) are satisfied if

$$S(\tau)u - K(\tau)v = -S(-\tau)u - K(-\tau)v, \tag{12}$$

$$-K(\tau)u - S(\tau)v = -K(-\tau)u + S(-\tau)v, \tag{13}$$

$$-\kappa_\tau(u,v,\tau) = \kappa_\tau(u,-v,-\tau). \tag{14}$$

The first two conditions are satified if the following symmetry conditions are fulfilled:

$$S(-\tau) = -S(\tau), \quad K(-\tau) = K(\tau). \tag{15}$$

From (10),

$$\kappa_\tau(u, -v, -\tau) = \frac{1}{2}\left(u^T K'(-\tau)u - u^T S'(-\tau)v - v^T S'^T(-\tau)u + v^T K'(-\tau)v\right).$$

The third condition for ρ-reversibility, (14), is thus satisfied if

$$K'(-\tau) = -K'(\tau), \quad S'(-\tau) = S'(\tau),$$

which is a consequence of the symmetry conditions (15).

We summarize our result in the following lemma.

Lemma 1. *The autonomous Hamiltonian system* (9) *is ρ-reversible if and only if the symmetry conditions* (15) *are satisfied.*

2 Time integration

We consider integrating (3) with a time-dependent forcing,

$$\begin{bmatrix} \dot{u} \\ \dot{v} \end{bmatrix} = \begin{bmatrix} S(t) & -K(t) \\ K(t) & S(t) \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} + \begin{bmatrix} F_u(t) \\ F_v(t) \end{bmatrix}. \tag{16}$$

Here, $u \in \mathbb{R}^N$ and $v \in \mathbb{R}^N$; $K = K^T$ and $S = -S^T$ are real-valued $N \times N$ matrices. To solve (16) numerically, we discretize time on a grid with $t_n = n\delta_t$, $n = 0, 1, 2, , \ldots$. Here, the time step (δ_t) is constant, but this assumption can be relaxed. We denote the numerical solution $u^n \approx u(t_n)$ and $v^n \approx v(t_n)$. In general, $S(t) \neq 0$ and the Hamiltonian system is non-separable. Givent (u^n, v^n), the Stromer-Verlet scheme evolves the solution by

$$\begin{aligned}
\left(I - \frac{\delta_t}{2}S^n\right)\ell_1 &= K^n u^n + S^n v^n + F_v^n, \\
v^{n+1/2} &= v^n + \frac{\delta_t}{2}\ell_1, \\
\kappa_1 &= S^{n+1/2}u^n - K^{n+1/2}v^{n+1/2} + F_u^{n+1/2}, \\
\left(I - \frac{\delta_t}{2}S^{n+1/2}\right)\kappa_2 &= S^{n+1/2}\left(u^n + \frac{\delta_t}{2}\kappa_1\right) - K^{n+1/2}v^{n+1/2} + F_u^{n+1/2}, \\
u^{n+1} &= u^n + \frac{\delta_t}{2}\left(\kappa_1 + \kappa_2\right), \\
\ell_2 &= K^{n+1}u^{n+1} + S^{n+1}v^{n+1/2} + F_v^{n+1}, \\
v^{n+1} &= v^n + \frac{\delta_t}{2}\left(\ell_1 + \ell_2\right).
\end{aligned}$$

If v^n is not needed, we can re-organize the scheme to instead start from $(u^n, v^{n-1/2})$,

$$
\begin{aligned}
\widetilde{\ell}_2 &= K^n u^n + S^n v^{n-1/2} + F_v^n, \\
\left(I - \frac{\delta_t}{2} S^n\right) \ell_1 &= K^n u^n + S^n \left(v^{n-1/2} + \frac{\delta_t}{2} \widetilde{\ell}_2\right) + F_v^n, \\
v^{n+1/2} &= v^{n-1/2} + \frac{\delta_t}{2} \left(\widetilde{\ell}_2 + \ell_1\right), \\
\kappa_1 &= S^{n+1/2} u^n - K^{n+1/2} v^{n+1/2} + F_u^{n+1/2}, \\
\left(I - \frac{\delta_t}{2} S^{n+1/2}\right) \kappa_2 &= S^{n+1/2} \left(u^n + \frac{\delta_t}{2} \kappa_1\right) - K^{n+1/2} v^{n+1/2} + F_u^{n+1/2}, \\
u^{n+1} &= u^n + \frac{\delta_t}{2} \left(\kappa_1 + \kappa_2\right),
\end{aligned}
$$

We note that the scheme becomes explicit when $S(t) = 0$. In this case the scheme simplifies significantly because $\widetilde{\ell}_2 = \ell_1$ and $\kappa_1 = \kappa_2$.

The above Stromer-Verlet scheme is second order accurate, symplectic and time reversible. By using a compositional technique where each time-step is decomposed into several sub-steps, the order of accuracy can be raised. Fourth order accuracy can be obtained with three sub-steps, sixth order with seven or nine sub-steps, and eight order requires at least fifteen sub-steps, see Harirer et al. [1] for further details.

References

[1] E. Hairer, C. Lubich, and G. Wanner. *Geometric Numerical Integration*. Number 31 in Springer series in computational mathematics. Springer-Verlag, Heidelberg, 2nd edition, 2006.