Solving the vectorized Liouville-von-Neumann equations for the real and imaginary part of the density matrix $\rho = u + iv$:

$$\begin{bmatrix} \dot{u} \\ \dot{v} \end{bmatrix} = \begin{bmatrix} A(t) & -B(t) \\ B(t) & A(t) \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} \tag{1}$$

with $A^T = -A, B^T = B$.

1 Backward-Euler

Compute u^{n+1}, v^{n+1} from

$$\begin{bmatrix} u^{n+1} \\ v^{n+1} \end{bmatrix} = \begin{bmatrix} I - \delta t A^{n+1} & \delta t B^{n+1} \\ -\delta t A^{n+1} & I - \delta t B^{n+1} \end{bmatrix}^{-1} \begin{bmatrix} u^n \\ v^n \end{bmatrix} \tag{2}$$

2 Stromer-Verlet

(Including forcing F_u, F_v). Compute u^{n+1}, v^{n+1} from

$$\left(I - \frac{\delta t}{2} A^n\right) \ell_1 = B^n u^n + A^n v^n + F_v^n, \tag{3}$$

$$v^{n+1/2} = v^n + \frac{\delta t}{2} \ell_1, \tag{4}$$

$$\kappa_1 = A^{n+1/2} u^n - B^{n+1/2} v^{n+1/2} + F_u^{n+1/2}, \tag{5}$$

$$\left(I - \frac{\delta t}{2} A^{n+1/2}\right) \kappa_2 = A^{n+1/2} \left(u^n + \frac{\delta t}{2} \kappa_1\right) - B^{n+1/2} v^{n+1/2} + F_u^{n+1/2}, \tag{6}$$

$$u^{n+1} = u^n + \frac{\delta t}{2} \left(\kappa_1 + \kappa_2\right), \tag{7}$$

$$\ell_2 = B^{n+1} u^{n+1} + A^{n+1} v^{n+1/2} + F_v^{n+1}, \tag{8}$$

$$v^{n+1} = v^n + \frac{\delta t}{2} \left(\ell_1 + \ell_2\right). \tag{9}$$

Neglecting F_u, F_v, the matrix notation of one time-step is

$$\begin{bmatrix} u^{n+1} \\ v^{n+1} \end{bmatrix} = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \begin{bmatrix} u^n \\ v^n \end{bmatrix} \tag{10}$$

with

$$A_{11} = I - \frac{\delta t^2}{2^2} B^n (I - \frac{\delta t}{2} A^{n+\frac{1}{2}})^{-1} B^{n+\frac{1}{2}} \tag{11}$$

$$+ \frac{\delta t}{2} A^n \tag{12}$$

$$- \frac{\delta t^2}{2^2} (I - \frac{\delta t}{2} A^{n+1})^{-1} B^{n+1} (I - \frac{\delta t}{2} A^{n+\frac{1}{2}})^{-1} B^{n+\frac{1}{2}} \tag{13}$$

$$+ \frac{\delta t}{2} (I - \frac{\delta t}{2} A^{n+1})^{-1} A^{n+1} \tag{14}$$

$$- \frac{\delta t^3}{2^3} (I - \frac{\delta t}{2} A^{n+1})^{-1} A^{n+1} B^n (I - \frac{\delta t}{2} A^{n+\frac{1}{2}})^{-1} B^{n+\frac{1}{2}} \tag{15}$$

$$+ \frac{\delta t^2}{2^2} (I - \frac{\delta t}{2} A^{n+1})^{-1} A^{n+1} A^n \tag{16}$$

$$A12 = -\frac{\delta t}{2} B^n \tag{17}$$

$$- \frac{\delta t^2}{2^2} B^n (I - \frac{\delta t}{2} A^{n+\frac{1}{2}})^{-1} A^{n+\frac{1}{2}} \tag{18}$$

$$- \frac{\delta t}{2} (I - \frac{\delta t}{2} A^{n+1})^{-1} B^{n+1} \tag{19}$$

$$- \frac{\delta t^2}{2^2} (I - \frac{\delta t}{2} A^{n+1})^{-1} B^{n+1} (I - \frac{\delta t}{2} A^{n+\frac{1}{2}})^{-1} A^{n+\frac{1}{2}} \tag{20}$$

$$- \frac{\delta t^2}{2^2} (I - \frac{\delta t}{2} A^{n+1})^{-1} A^{n+1} B^n \tag{21}$$

$$- \frac{\delta t^3}{2^3} (I - \frac{\delta t}{2} A^{n+1})^{-1} A^{n+1} B^n (I - \frac{\delta t}{2} A^{n+\frac{1}{2}})^{-1} A^{n+\frac{1}{2}} \tag{22}$$

$$A21 = \frac{\delta t}{2} B^{n+\frac{1}{2}} \tag{23}$$

$$- \frac{\delta t^3}{2^3} B^{n+\frac{1}{2}} B^n (I - \frac{\delta t}{2} A^{n+\frac{1}{2}})^{-1} B^{n+\frac{1}{2}} \tag{24}$$

$$+ \frac{\delta t^2}{2^2} B^{n+\frac{1}{2}} A^n \tag{25}$$

$$- \frac{\delta t^3}{2^3} B^{n+\frac{1}{2}} (I - \frac{\delta t}{2} A^{n+1})^{-1} B^{n+1} (I - \frac{\delta t}{2} A^{n+\frac{1}{2}})^{-1} B^{n+\frac{1}{2}} \tag{26}$$

$$+ \frac{\delta t^2}{2^2} B^{n+\frac{1}{2}} (I - \frac{\delta t}{2} A^{n+1})^{-1} A^{n+1} \tag{27}$$

$$- \frac{\delta t^4}{2^4} B^{n+\frac{1}{2}} (I - \frac{\delta t}{2} A^{n+1})^{-1} A^{n+1} B^n (I - \frac{\delta t}{2} A^{n+\frac{1}{2}})^{-1} B^{n+\frac{1}{2}} \tag{28}$$

$$+ \frac{\delta t^3}{2^3} B^{n+\frac{1}{2}} (I - \frac{\delta t}{2} A^{n+1})^{-1} A^{n+1} A^n \tag{29}$$

$$+ \frac{\delta t^2}{2^2} A^{n+\frac{1}{2}} (I - \frac{\delta t}{2} A^{n+\frac{1}{2}})^{-1} B^{n+\frac{1}{2}} \tag{30}$$

$$+ \frac{\delta t}{2} (I - \frac{\delta t}{2} A^{n+\frac{1}{2}})^{-1} B^{n+\frac{1}{2}} \tag{31}$$

$$A_{22} = I - \frac{\delta t^2}{2^2} B^{n+\frac{1}{2}} B^n \tag{32}$$

$$- \frac{\delta t^3}{2^3} B^{n+\frac{1}{2}} B^n (I - \frac{\delta t}{2} A^{n+\frac{1}{2}})^{-1} A^{n+\frac{1}{2}} \tag{33}$$

$$- \frac{\delta t^2}{2^2} B^{n+\frac{1}{2}} (I - \frac{\delta t}{2} A^{n+1})^{-1} B^{n+1} \tag{34}$$

$$- \frac{\delta t^3}{2^3} B^{n+\frac{1}{2}} (I - \frac{\delta t}{2} A^{n+1})^{-1} B^{n+1} (I - \frac{\delta t}{2} A^{n+\frac{1}{2}})^{-1} A^{n+\frac{1}{2}} \tag{35}$$

$$- \frac{\delta t^3}{2^3} B^{n+\frac{1}{2}} (I - \frac{\delta t}{2} A^{n+1})^{-1} A^{n+1} B^n \tag{36}$$

$$- \frac{\delta t^4}{2^4} B^{n+\frac{1}{2}} (I - \frac{\delta t}{2} A^{n+1})^{-1} A^{n+1} B^n (I - \frac{\delta t}{2} A^{n+\frac{1}{2}})^{-1} A^{n+\frac{1}{2}} \tag{37}$$

$$+ \frac{\delta t}{2} A^{n+\frac{1}{2}} \tag{38}$$

$$+ \frac{\delta t^2}{2^2} A^{n+\frac{1}{2}} (I - \frac{\delta t}{2} A^{n+\frac{1}{2}})^{-1} A^{n+\frac{1}{2}} \tag{39}$$

$$+ \frac{\delta t}{2} (I - \frac{\delta t}{2} A^{n+\frac{1}{2}})^{-1} A^{n+\frac{1}{2}} \tag{40}$$

3 Testproblems

3.1 1 oscillator system with 2 levels - Case 1

Consider a 1 oscillator system with 2 levels $\Rightarrow a = a_1 = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$, $N = 2^1 = 2$. Consider the Hamiltonian

$$\begin{aligned} H(t) &= f_1(t)(a_1 + a_1^\dagger) \\ \text{with} \quad f_1(t) &= \frac{1}{4}(1 - \cos(wt)), \quad a_1 + a_1^\dagger = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \end{aligned}$$

when solving the Liouville-von-Neumann equation for the density matrix $\rho \in \mathbb{C}^{2\times 2}$. After vectorization vec$\rho =: \tilde{\rho} \in \mathbb{C}^4$ we solve

$$\begin{aligned} \dot{\tilde{\rho}} &= -i(I_2 \otimes H - H^T \otimes I_2)\tilde{\rho} \\ &= i f_1(t) \underbrace{\begin{pmatrix} 0 & -1 & 1 & 0 \\ -1 & 0 & 0 & 1 \\ 1 & 0 & 0 & -1 \\ 0 & 1 & -1 & 0 \end{pmatrix}}_{=:B_0} \tilde{\rho} \end{aligned}$$

Hence, $A(t) = 0 \in \mathbb{R}^{4\times 4}$ and $B(t) = f_1(t)B_0$ for the system in (1).

3.2 1 oscillator system with 2 levels - Case 2

Consider a 1 oscillator system with 2 levels $\Rightarrow a = a_1 = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$, $N = 2^1 = 2$. Consider the Hamiltonian

$$\begin{aligned} H(t) &= i g_1(t)(a_1 - a_1^\dagger) \\ \text{with} \quad g_1(t) &= \frac{1}{4}(1 - \sin(wt)), \quad a_1 - a_1^\dagger = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \end{aligned}$$

when solving the Liouville-von-Neumann equation for the density matrix $\rho \in \mathbb{C}^{2\times 2}$. After vectorization vec$\rho =: \tilde{\rho} \in \mathbb{C}^4$ we solve

$$\begin{aligned}\dot{\tilde{\rho}} &= -i(I_2 \otimes H - H^T \otimes I_2)\tilde{\rho} \\ &= g_1(t) \underbrace{\begin{pmatrix} 0 & 1 & -1 & 0 \\ -1 & 0 & 0 & -1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & -1 & 0 \end{pmatrix}}_{=:A_0} \tilde{\rho}\end{aligned}$$

Hence, $A(t) = g_1(t)A_0$ and $B(t) = 0$ for the system in (1).

3.3 2 oscillators, 2 levels

Consider 2 oscillator system with $n = 2$ levels $\Rightarrow a_1 = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$ and $a = a_1 \otimes I_2, b = I_2 \otimes a_1$.

Consider the Hamiltonian

$$\begin{aligned}H(t) &:= f_1(t)(a + a^\dagger) + ig_1(t)(a - a^\dagger) \\ &= \begin{pmatrix} 0 & ig_1(t) & f_1(t) & 0 \\ -ig_1(t) & 0 & 0 & f_1(t) \\ f_1(t) & 0 & 0 & ig_1(t) \\ 0 & f_1(t) & -ig_1(t) & 0 \end{pmatrix}\end{aligned}$$

where

$$f_1(t) := \frac{1}{4}(1 - \cos(wt)), \quad g_1(t) := \frac{1}{4}(1 - \sin(wt))$$

Vectorization and real/imaginary splitting gives the following system matrices:

$$
\begin{aligned}
A(t) &= I_4 \otimes Im(H) - Im(H)^T \otimes I_4 \\
&= g_1(t)\left(I_4 \otimes (a - a^\dagger) - (a - a^\dagger)^T \otimes I_4\right) \\
&= g_1(t) \left(\begin{array}{cccc|cccc|cccc|cccc}
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
-1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
\hline
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\
\hline
-1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\
\hline
0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0
\end{array}\right)
\end{aligned}
$$

$$
\begin{aligned}
B(t) &= -I_4 \otimes Re(H) + Re(H)^T \otimes I_4 \\
&= f_1(t) \left(-I_4 \otimes (a + a^\dagger) + (a + a^\dagger)^T \otimes I_4 \right) \\
&= f_1(t) \left(\begin{array}{cccc|cccc|cccc|cccc}
0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
-1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
\hline
0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\
\hline
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\
\hline
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0
\end{array} \right)
\end{aligned}
$$