EXERCISE 8.1

a)

discrete Hamiltonian:

EF

$$\mathcal{H}^{n+1} = \frac{1}{2}\left((x^{n+1})^2+(y^{n+1})^2\right) = \frac{1}{2}\left((x^n+hy^n)^2+(y^n-hx^n)^2\right)$$

at $t=t^{n+1}$

$$= \frac{1}{2}\left((x^n)^2+\cancel{2hx^ny^n}+h^2(y^n)^2+(y^n)^2-\cancel{2hx^ny^n}+h^2(x^n)^2\right)$$

$$= \frac{1}{2}\left((x^n)^2+(y^n)^2\right)+\frac{1}{2}h^2\left((x^n)^2+(y^n)^2\right)$$

$$= (1+h^2)\frac{1}{2}\left((x^n)^2+(y^n)^2\right)$$

$$= (1+h^2)\,\mathcal{H}^n$$

>1 at $t=t^n$

$> \mathcal{H}^n$

$\boxed{\text{energy increases}}$

(must stay constant)

b)

EB

$$\Rightarrow \underbrace{\frac{1}{2}\left((x^{n+1})^2+(y^{n+1})^2\right)}_{\mathcal{H}^{n+1}} = --- = \frac{1}{2}\frac{(x^n)^2+(y^n)^2}{(1+h^2)^2}+\frac{h^2}{2}\frac{(x^n)^2+(y^n)^2}{(1+h^2)^2}$$

$$= \frac{1}{2}\frac{1+h^2}{(1+h^2)^2}\left((x^n)^2+(y^n)^2\right)$$

$$= \frac{1}{2}\frac{(x^n)^2+(y^n)^2}{1+h^2} = \frac{\mathcal{H}^n}{1+h^2} < \mathcal{H}^n$$

energy decreases

(must stay constant)

c) implicit midpoint

inverse matrix $\Rightarrow$

$$\begin{pmatrix} x^{n+1} \\ y^{n+1} \end{pmatrix} = \frac{1}{1+\frac{h^2}{4}} \begin{pmatrix} 1 & \frac{h}{2} \\ -\frac{h}{2} & 1 \end{pmatrix} \begin{pmatrix} x^n + \frac{h}{2}y^n \\ y^n - \frac{h}{2}x^n \end{pmatrix}$$

$$= \frac{1}{1+\frac{h^2}{4}} \begin{pmatrix} x^n + \frac{h}{2}y^n + \frac{h}{2}y^n - \frac{h^2}{4}x^n \\ -\frac{h}{2}x^n - \frac{h^2}{4}y^n + y^n - \frac{h}{2}x^n \end{pmatrix}$$

$$= \frac{1}{1+\frac{h^2}{4}} \begin{pmatrix} (1-\frac{h^2}{4})x^n + hy^n \\ (1-\frac{h^2}{4})y^n - hx^n \end{pmatrix}$$

$$\mathcal{H}^{n+1} = \frac{1}{2}((x^{n+1})^2 + (y^{n+1})^2)$$

$$= \frac{1}{2}\frac{1}{(1+\frac{h^2}{4})^2}\Big\{(1-\frac{h^2}{4})^2(x^n)^2 + 2h\cancel{(1-\frac{h^2}{4})x^n y^n} + h^2(y^n)^2$$
$$+ (1-\frac{h^2}{4})^2(y^n)^2 - 2h(1-\frac{h^2}{4})x^n y^n + h^2(x^n)^2\Big\}$$

$$= \frac{1}{2}\frac{1}{(1+\frac{h^2}{4})^2}\Big\{(1-\frac{h^2}{4})^2((x^n)^2+(y^n)^2) + h^2((x^n)^2+(y^n)^2)\Big\}$$

$$= \frac{1}{2}\frac{1}{(1+\frac{h^2}{4})^2}\Big\{\Big[(1-\frac{h^2}{4})^2 + h^2\Big]((x^n)^2+(y^n)^2)\Big\}$$

$$= \frac{1}{2}\cdot \underbrace{\boxed{\frac{1-\frac{h^2}{2}+\frac{h^4}{16}+h^2}{1+\frac{h^2}{2}+\frac{h^4}{16}}}}_{=1}((x^n)^2+(y^n)^2) = \frac{1}{2}((x^n)^2+(y^n)^2)$$

$$= \mathcal{H}^n$$

discrete Hamiltonian stays constant in time!

$\boxed{8.2}$

$$\begin{cases} x' = y \\ y' = -x \end{cases}$$

$$\begin{cases} x^{n+1} - x^n = \dfrac{1-\cos(\Delta t)}{\sin(\Delta t)} (y^{n+1} + y^n) \overset{\text{def.}}{=} \alpha \cdot (y^{n+1} + y^n) \\ y^{n+1} - y^n = \dfrac{1-\cos(\Delta t)}{\sin(\Delta t)} \cdot -(x^{n+1} + x^n) = -\alpha (x^{n+1} + x^n) \end{cases}$$

$$\underbrace{\begin{pmatrix} 1 & -\alpha \\ \alpha & 1 \end{pmatrix}}_{\det = 1+\alpha^2} \begin{pmatrix} x^{n+1} \\ y^{n+1} \end{pmatrix} = \begin{pmatrix} x^n + \alpha y^n \\ y^n - \alpha x^n \end{pmatrix}$$

$$\text{inverse} = \frac{1}{1+\alpha^2} \begin{pmatrix} 1 & \alpha \\ -\alpha & 1 \end{pmatrix}$$

$$\Rightarrow \begin{pmatrix} x^{n+1} \\ y^{n+1} \end{pmatrix} = \frac{1}{1+\alpha^2} \begin{pmatrix} 1 & \alpha \\ -\alpha & 1 \end{pmatrix} \begin{pmatrix} x^n + \alpha y^n \\ y^n - \alpha x^n \end{pmatrix}$$

$$\Rightarrow \begin{pmatrix} x^{n+1} \\ y^{n+1} \end{pmatrix} = \frac{1}{1+\alpha^2} \begin{pmatrix} (1-\alpha^2) x^n + 2\alpha y^n \\ -2\alpha x^n + (1-\alpha^2) y^n \end{pmatrix}$$

and $(x^{n+1})^2 + (y^{n+1})^2 \overset{?}{=} \cdots = \cdots = (x^n)^2 + (y^n)^2$

8.4

(a)

The governing equations are then

$$\frac{dp_1}{dt} = -\frac{q_1}{(q_1^2+q_2^2)^{3/2}},$$

$$\frac{dp_2}{dt} = -\frac{q_2}{(q_1^2+q_2^2)^{3/2}},$$

$$\frac{dq_1}{dt} = p_1,$$

$$\frac{dq_2}{dt} = p_2.$$

(b)

$$\frac{dH}{dt} = \frac{\partial H}{\partial p_1}\dot{p}_1 + \frac{\partial H}{\partial p_2}\dot{p}_2 + \frac{\partial H}{\partial q_1}\dot{q}_1 + \frac{\partial H}{\partial q_2}\dot{q}_2$$

$$= \cdots = 0$$

8.5

(a)

$$dA_{\square} = \begin{vmatrix} x & y & 1 \\ x+dx & y & 1 \\ x & y+dy & 1 \end{vmatrix} = \begin{vmatrix} x & y & 1 \\ dx & 0 & 0 \\ 0 & dy & 0 \end{vmatrix} = dx * dy,$$

as expected.

(b)

Now consider a small parallelogram with three corners (x_1, y_1), (x_2, y_2) and (x_3, y_3), and area

$$A = \begin{vmatrix} x_1 & y_1 & 1 \\ x_2 & y_2 & 1 \\ x_3 & y_3 & 1 \end{vmatrix}$$

so that

$$\frac{dA_\diamond}{dt} = \begin{vmatrix} \dot{x}_1 & \dot{y}_1 & 0 \\ x_2 & y_2 & 1 \\ x_3 & y_3 & 1 \end{vmatrix} + \begin{vmatrix} x_1 & y_1 & 1 \\ \dot{x}_2 & \dot{y}_2 & 0 \\ x_3 & y_3 & 1 \end{vmatrix} + \begin{vmatrix} x_1 & y_1 & 1 \\ x_2 & y_2 & 1 \\ \dot{x}_3 & \dot{y}_3 & 0 \end{vmatrix}$$

Hence

$$\frac{dA_\diamond}{dt} = \begin{vmatrix} y_1 & -x_1 & 0 \\ x_2 & y_2 & 1 \\ x_3 & y_3 & 1 \end{vmatrix} + \begin{vmatrix} x_1 & y_1 & 1 \\ y_2 & -x_2 & 0 \\ x_3 & y_3 & 1 \end{vmatrix} + \begin{vmatrix} x_1 & y_1 & 1 \\ x_2 & y_2 & 1 \\ y_3 & -x_3 & 0 \end{vmatrix}$$

and evaluating the determinants and summing,

$$\frac{dA_\diamond}{dt} = 0.$$

and the mapping is area preserving.

(c)

Now look at a numerical method, here we consider Euler's method, where in one time step of size Δt, if we take three points (X_1, Y_1), (X_2, Y_2), (X_3, Y_3),

$$X_r \to X_r + \Delta t Y_r, \quad Y_r \to Y_r - \Delta t X_r, \quad r = 1, 2, 3,$$

with area

$$A = \begin{vmatrix} X_1 & Y_1 & 1 \\ X_2 & Y_2 & 1 \\ X_3 & Y_3 & 1 \end{vmatrix}$$

Algebra can be simplified by choosing points (X_1, Y_1), $(X_1 + h, Y_1)$, $(X_1, Y_1 + k)$ and denote the initial element of area as $A_0 = hk$. In one timestep the vertices change according to Euler's method to give area

$$A_1 = A(\Delta t) = \begin{vmatrix} X_1 + \Delta t Y_1 & Y_1 - \Delta t X_1 & 1 \\ X_1 + h + \Delta t Y_1 & Y_1 - \Delta t (X_1 + h) & 1 \\ X_1 + \Delta t (Y_1 + k) & Y_1 + k - \Delta t X_1 & 1 \end{vmatrix}$$

or

$$A_1 = \begin{vmatrix} X_1 + \Delta t Y_1 & Y_1 - \Delta t X_1 & 1 \\ h & -\Delta t h & 0 \\ \Delta t k & k & 0 \end{vmatrix},$$

and thus

$$\underline{A_1 = (1 + \Delta t^2)hk.}$$

so that explicit Euler's method will not preserve area and elements of area will increase exponentially.

(d) after a long(er) calculation than in (c) .... $\Rightarrow$ -- $\Rightarrow$ $A_1 = hk = A_0$


(sorry --)

area is preserved

(e)

$$\hat{\mathcal{H}}_{n+1} = \underbrace{\frac{1}{2}(x_{n+1}^2 + y_{n+1}^2)}_{H(x_{n+1}, y_{n+1})} - \underline{\frac{1}{2}\Delta t . x_{n+1} y_{n+1}}$$

$$\hat{\mathcal{H}}_n = \underbrace{\frac{1}{2}(x_n^2 + y_n^2)}_{H(x_n, y_n)} - \underline{\frac{1}{2}\Delta t . x_n y_n}$$

use the two discrete formulas in the exercise .... .. $\Rightarrow$ $\hat{\mathcal{H}}_{n+1} = \hat{\mathcal{H}}_n$

(not: $\mathcal{H}_{n+1} = \mathcal{H}_n$)

This scheme also does not leave the original Hamiltonian $H(x,y)$ unaltered, but it does preserve a modified Hamiltonian

$$H(x,y) = \frac{1}{2}(x^2 + y^2) - \frac{1}{2}\Delta t xy = H(x,y) - \frac{1}{2}\Delta t xy$$

This is called a symplectic scheme and it is a general property of symplectic schemes that while not preserving the original Hamiltonian they do exactly preserve an approximate Hamiltonian which, in the limit of $\Delta t \to 0$, restores the original Hamiltonian

8.6

$$u_{tt} = u_{xx} \quad , \quad \mathcal{H}_1 = \frac{1}{2}\int_\Omega [u_x^2 + v^2]\,dx$$

(linear wave equation

$$u_t = v,\ v_t = u_{tt} = u_{xx} \Rightarrow \begin{cases} \dfrac{\partial u}{\partial t} = \dfrac{\delta \mathcal{H}}{\delta v} = v \\[2mm] \dfrac{\partial v}{\partial t} = -\dfrac{\delta \mathcal{H}}{\delta u} = u_{xx} \end{cases}$$

$$\Updownarrow$$

$$\begin{pmatrix} u \\ v \end{pmatrix}_t = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \frac{\delta \mathcal{H}}{\delta u} \\ \frac{\delta \mathcal{H}}{\delta v} \end{pmatrix} \overset{\text{def}}{=} \mathcal{J} \begin{pmatrix} \frac{\delta \mathcal{H}}{\delta u} \\ \frac{\delta \mathcal{H}}{\delta v} \end{pmatrix}$$

Nonlinear wave equation

$$u_{tt} - u_{xx} + V'(u) = 0$$

$$\mathcal{H} = \int \left[\frac{1}{2} p^2 + \frac{1}{2} q_x^2 + V(q)\right] dx$$

$$\begin{matrix} u = q \\ p = q_t \end{matrix} \Rightarrow \begin{pmatrix} q \\ p \end{pmatrix}_t = \underset{\sim}{\mathcal{J}} \begin{pmatrix} \frac{\delta \mathcal{H}}{\delta q} \\ \frac{\delta \mathcal{H}}{\delta p} \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} p \\ q_{xx} - V'(q) \end{pmatrix}$$

8.7

Extended KdV5 :

$$u_t + \frac{2}{15}u_{5x} + uu_{3x} + 3uu_x + 2u_{xx}u_x = 0$$

$$\hookrightarrow\ u_t = \mathcal{J}\frac{\delta\mathcal{H}}{\delta u} = -\frac{\partial}{\partial x}\Big[\frac{3}{2}u^2 + \frac{1}{3}u_{xx} + \frac{2}{15}u_{4x} + \frac{1}{2}u_x^2 - (uu_x)_x$$

"non-canonical form"

$$\mathcal{H} = \int_\Omega \Big[\frac{1}{3}u^3 - 3u_x^2 + \frac{1}{15}u_{xx}^2 + \frac{1}{2}uu_x^2\Big]dx$$

$$u_t + \frac{2}{15}u_{5x} + uu_{3x} - bu_{3x} + 3uu_x + 2u_xu_{xx} = 0$$

$$\Updownarrow$$

$$u_t + \frac{\partial}{\partial x}\Big[\underbrace{\frac{2}{15}u_{4x} - bu_{xx} + \frac{3}{2}u^2 - \frac{1}{2}u_x^2 + (uu_x)_x}_{(*)}\Big] = 0$$

$$\Updownarrow$$

$$u_t + \frac{\partial}{\partial x}\Big[\frac{\delta\mathcal{H}}{\delta u}\Big] = 0$$

Take $b=0$

met $\mathcal{H} = \int_\Omega \Big(\frac{1}{15}u_{xx}^2 + \frac{1}{2}u^3 + \frac{b}{2}u_x^2 - \frac{1}{2}uu_x^2\Big)dx$

$$:= \int_\Omega f(u, u_x, u_{xx})\,dx$$

variational derivative

$$\frac{\delta\mathcal{H}}{\delta u} := \frac{\partial f}{\partial u} - \frac{d}{dx}\frac{\partial f}{\partial u_x} + \frac{d^2}{dx^2}\frac{\partial f}{\partial u_{xx}}$$

$$= \frac{3}{2}u^2 - \frac{1}{2}u_x^2 - \frac{d}{dx}\big(bu_x - uu_x\big) + \frac{d^2}{dx^2}\Big(\frac{2}{15}u_{xx}\Big)$$

$$= \frac{3}{2}u^2 - \frac{1}{2}u_x^2 - bu_{xx} + (uu_x)_x + \frac{2}{15}u_{4x}$$

$$\equiv (*)$$

8.9

$$u_t - 6uu_x + \underset{\substack{\| \\ u_{xxx}}}{u_{3x}} = 0$$ skew-symmetric operator

$$\Leftrightarrow u_t = \mathcal{J}\frac{\delta\mathcal{H}}{\delta u} = \frac{\partial}{\partial x}\left[3u^2 - u_{xx}\right]$$

$$\mathcal{J} = \frac{\partial}{\partial x}, \quad \mathcal{H} = \int_\Omega \left[\tfrac{1}{2}u_x^2 + u^3\right]dx$$

$$\frac{\delta\mathcal{H}}{\delta u} = \frac{\partial}{\partial u}\left(\tfrac{1}{2}u_x^2 + u^3\right) - \frac{d}{dx}\frac{\partial}{\partial u_x}\left(\tfrac{1}{2}u_x^2 + u^3\right)$$
$$= 3u^2 - \frac{d}{dx}(u_x) = 3u^2 - u_{xx}$$

PROPERTY

* $\{T,S\} \overset{\text{def}}{=} \int_\Omega \frac{\delta T}{\delta u}\mathcal{J}\frac{\delta S}{\delta u}dx \Rightarrow$

Define: Poisson bracket

$$\{T,S\} = \int_\Omega \frac{\delta T}{\delta u}\frac{\partial}{\partial x}\left(\frac{\delta S}{\delta u}\right)dx$$
$$= -\int_\Omega \frac{\delta S}{\delta u}\frac{\partial}{\partial x}\left(\frac{\delta T}{\delta u}\right)dx$$
$$= -\int_\Omega \frac{\delta S}{\delta u}\mathcal{J}\frac{\delta T}{\delta u}dx = -\{S,T\}$$

skew symmetric

en dus $\{\mathcal{H},\mathcal{H}\} = -\{\mathcal{H},\mathcal{H}\}$
$\Rightarrow \{\mathcal{H},\mathcal{H}\} = 0$

* $\mathcal{H} \overset{\text{def}}{=} \int_\Omega f(u, u_x, u_{xx}, \ldots)\,dx \Rightarrow \frac{d\mathcal{H}}{dt} = \frac{d}{dt}\int_\Omega f\,dx = \int_\Omega \frac{d}{dt}f\,dx =$

in general:

$$= \int_\Omega \left(\frac{\partial f}{\partial u}u_t + \frac{\partial f}{\partial u_x}u_{xt} + \frac{\partial f}{\partial u_{xx}}u_{xxt} + \ldots\right)dx$$
$$= \int_\Omega \left(\frac{\partial f}{\partial u}u_t + \frac{\partial f}{\partial u_x}(u_t)_x + \frac{\partial f}{\partial u_{xx}}(u_t)_{xx} + \ldots\right)dx$$
$$= \int_\Omega \left(\frac{\partial f}{\partial u}u_t - \frac{d}{dx}\frac{\partial f}{\partial u_x}u_t + \frac{d^2}{dx^2}\frac{\partial f}{\partial u_{xx}}u_t + \ldots\right)dx$$
$$= \int_\Omega \left(\frac{\partial f}{\partial u} - \frac{d}{dx}\frac{\partial f}{\partial u_x} + \frac{d^2}{dx^2}\frac{\partial f}{\partial u_{xx}} + \ldots\right)u_t\,dx$$
$$= \int_\Omega \frac{\delta\mathcal{H}}{\delta u}u_t\,dx$$
$$= \int_\Omega \frac{\delta\mathcal{H}}{\delta u}\mathcal{J}\frac{\delta\mathcal{H}}{\delta u}dx = \{\mathcal{H},\mathcal{H}\} = 0$$

8.10

Consider the non-linear Schrödinger equation (NLS), for complex-values function $\psi(t,x) = q(t,x) + ip(t,x)$ with real q and p:

$$i\psi_t = -\psi_{xx} - 2|\psi|^2\psi. \qquad (1)$$

(a) We will consider this function on a domain $x \in [0, L)$ with periodic boundary conditions. First, we will show that the NLS is a canonical Hamiltonian PDE, with Hamiltonian functional

$$\mathcal{H} = \int \frac{1}{2}|\psi_x|^2 - \frac{1}{2}|\psi|^4 dx. \qquad (2)$$

By $\psi(t,x) = q(t,x) + ip(t,x)$, we know that $|\psi|^2 = q^2 + p^2$ and $|\psi_x|^2 = p_x^2 + q_x^2$, so by substituting this in (2), we find:

$$\mathcal{H} = \int \frac{1}{2}(q_x^2 + p_x^2) - \frac{1}{2}(q^2 + p^2)^2 dx.$$

A canonical Hamiltonian PDE is of the form

$$\begin{pmatrix} q_t \\ p_t \end{pmatrix} = \mathcal{J}\begin{pmatrix} \frac{\delta\mathcal{H}[\psi]}{\delta q} \\ \frac{\delta\mathcal{H}[\psi]}{\delta p} \end{pmatrix}, \qquad (3)$$

for skew-symmetric matrix $\mathcal{J} = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}$. In our case, we have $\mathcal{J} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$. Let $h = \frac{1}{2}q_x^2 + p_x^2 - \frac{1}{2}(q^2 + p^2)^2$. For the variational derivative of $\mathcal{H}$, we find

$$\frac{\delta\mathcal{H}[\psi]}{\delta q} = \frac{\partial h}{\partial q} - \frac{\partial}{\partial x}\frac{\partial h}{\partial q_x} = -2q(q^2 + p^2) - \frac{\partial}{\partial x}q_x = -2q(q^2 + p^2) - q_{xx}.$$

$$\frac{\delta\mathcal{H}[\psi]}{\delta p} = \frac{\partial h}{\partial p} - \frac{\partial}{\partial x}\frac{\partial h}{\partial p_x} = -2p(q^2 + p^2) - \frac{\partial}{\partial x}p_x = -2p(q^2 + p^2) - p_{xx}.$$

We know that $i\psi_t = iq_t - p_t$, which should be equal to $i\frac{\delta\mathcal{H}[\psi]}{\delta p} + \frac{\delta\mathcal{H}[\psi]}{\delta q}$ to satisfy (3). We find:

$$\begin{aligned} i\frac{\delta\mathcal{H}[\psi]}{\delta p} + \frac{\delta\mathcal{H}[\psi]}{\delta q} &= -2ip(q^2 + p^2) - ip_{xx} - 2q(q^2 + p^2) - q_{xx} \\ &= -2(q + ip)(q^2 + p^2) - (q_{xx} + ip_{xx}) \\ &= -2\psi|\psi|^2 - \psi_{xx}. \end{aligned}$$

which indeed corresponds with our original equation (1).

It is now easy to see that the Hamiltonian functional is a conserved quantity. We have:

$$\frac{d}{dt}\mathcal{H} = \frac{\delta\mathcal{H}}{\delta q}\dot{q} + \frac{\delta\mathcal{H}}{\delta p}\dot{p} = -\dot{p}\dot{q} + \dot{q}\dot{p} = 0.$$

(b) The following quadratic integrals are conserved quantities as well.

$$\mathcal{N} = \int |\psi|^2 dx. \qquad \mathcal{M} = \int \psi\bar{\psi}_x dx.$$

We know that $|\psi|^2 = p^2 + q^2$. Using this, we find for $\mathcal{N}$:

$$\frac{\partial}{\partial t}\mathcal{N} = \frac{\partial}{\partial t}\int_0^L p^2 + q^2 dx = \int_0^L 2pp_t + 2qq_t dx.$$

Substituting $p_t = q_{xx} + 2q(q^2+p^2)$ and $q_t = -2p(q^2+p^2) - p_{xx}$, gives:

$$\frac{\partial}{\partial t}\mathcal{N} = 2\int_0^L 2pq(q^2+p^2) + pq_{xx} - 2pq(q^2+p^2) - qp_{xx}dx = 2\int_0^L pq_{xx} - qp_{xx}dx$$

From integration by parts, we find

$$\int_0^L pq_{xx}dx = [pq_x]_0^L - \int_0^L p_x q_x dx$$
$$\int_0^L qp_{xx}dx = [qp_x]_0^L - \int_0^L p_x q_x dx$$

By subtracting these two equations, we find

$$\frac{\partial}{\partial t}\mathcal{N} = 2[pq_x]_0^L - 2[qp_x]_0^L.$$

By the periodic boundary conditions, we have $p(t,0) = p(t,L)$ and $q(t,0) = q(t,L)$, so we find that $\frac{\partial}{\partial t}\mathcal{N} = 0$. This means that $\mathcal{N}$ is a conserved quantity. In a similar way, we find that $\frac{\partial}{\partial t}\mathcal{M} = 0$. First, we find for $\mathcal{M}$:

$$\begin{aligned}\mathcal{M} &= \int_0^L \bar{v}v_x dx = \int_0^L (q-ip)(q_x+ip_x)dx = \int_0^L qq_x + iqp_x - ipq_x + pp_x dx\\ &= \int_0^L \frac{1}{2}\frac{\partial}{\partial x}q^2 + \frac{1}{2}\frac{\partial}{\partial x}p^2 + i(qp_x - pq_x)dx = \frac{1}{2}[q^2+p^2]_0^L + i\int_0^L (qp_x - pq_x)dx\\ &= i\int_0^L (qp_x - pq_x)dx,\end{aligned}$$

where the last equality follows from the periodic boundary conditions. We have

$$\frac{\partial}{\partial t}\mathcal{M} = i\frac{\partial}{\partial t}\int_0^L qp_x - pq_x dx = i\int_0^L q_t p_x + qp_{xt} - p_t q_x - pq_{xt}dx$$

From integration by parts, we find

$$\int_0^L pq_{xt}dx = [pq_t]_0^L - \int_0^L q_t p_x dx. \qquad \int_0^L qp_{xt}dx = [qp_t]_0^L - \int_0^L p_t q_x dx.$$

This gives

$$\frac{\partial}{\partial t}\mathcal{M} = i\int_0^L q_t p_x - q_x p_t - p_t q_x + q_t p_x dx + [qp_t]_0^L - [pq_t]_0^L = 2i\int_0^L q_t p_x - p_t q_x dx.$$

by the periodicity. Substituting p_t and q_t gives

$$\begin{aligned}\frac{\partial}{\partial t}\mathcal{M} &= 2i\int_0^L -2(pp_x + qq_x)(p^2+q^2) - p_x p_{xx} + q_x q_{xx}dx.\\ &= 2i\int_0^L -\frac{\partial}{\partial x}(p^2+q^2) - \frac{\partial}{\partial x}\frac{(p_x)^2}{2} + \frac{\partial}{\partial x}\frac{(q_x)^2}{2}dx.\\ &= -2i([p^2+q^2]_0^L - i[p_x^2]_0^L + i[q_x^2]_0^L = 0.\end{aligned}$$

where the last equality follosw from the periodic boundary conditions. Therefore, we have that $\mathcal{M}$ is also a conserved quantity.

(c)

Spatial discretisation

We will construct a Hamiltonian spatial discretisation of the NLS equation. First, we need a grid. Let $x_i = i\Delta x$ for $i = 0, ..., N$ with $\Delta x = \frac{L}{N}$. Also, we introduce the notation $\psi_i(t) \approx \psi(t, x_i)$ for $i = 0, ..., N-1$ where $\psi_0 = \psi_N$ by the periodic boundary conditions. The discrete vector space V consists of the functions $v_i(t)$. We define our inner product as follows:

$$\langle u, v\rangle = \sum_{i=0}^{N-1} u_i^T v_i \Delta x.$$

Then the variational derivative is defined as:

$$\langle \frac{\delta F}{\delta u}, v\rangle = \lim_{\epsilon\to 0} \frac{1}{\epsilon}(F(u+\epsilon v) - F(u)),$$

for all $v \in V$. A Hamiltonian spatial discretisation means that we need to find H, an approximation of $\mathcal{H}$ and J, an approximation of $\mathcal{J}$ so that the discretisation is defined by $\dot{v}_t = J\frac{\delta H}{\delta v}$. The operator $\mathcal{J}$ is approximated by $J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$. We can find the variational derivates with respect to p and q. We have

$$H = \frac{1}{2}\sum_{i=0}^{N-1}[(\frac{q_{i+1}-q_i}{\Delta x})^2 + (\frac{p_{i+1}-p_i}{\Delta x})^2 - (q_i^2+p_i^2)^2]\Delta x.$$

We will derive $\frac{\delta H}{\delta q_i}$; then $\frac{\delta H}{\delta p_i}$ is similar due to the symmetry in H. We have

$$\begin{aligned}
\langle \frac{\delta H}{\delta q_i}, v\rangle &= \lim_{\epsilon\to 0}\frac{\Delta x}{2\epsilon}\sum_{i=0}^{N-1}[(\frac{q_{i+1}+\epsilon v_{i+1}-q_i-\epsilon v_i}{\Delta x})^2 + (\frac{p_{i+1}-p_i}{\Delta x})^2 - ((q_i+\epsilon v_i)^2+p_i^2)^2 \\
&\quad - (\frac{q_{i+1}-q_i}{\Delta x})^2 + (\frac{p_{i+1}-p_i}{\Delta x})^2 + (q_i^2+p_i^2)^2] \\
&= \lim_{\epsilon\to 0}\frac{\Delta x}{2\epsilon}\sum_{i=0}^{N-1}[(\frac{q_{i+1}-q_i+\epsilon(v_{i+1}-v_i)}{\Delta x})^2 + (\frac{p_{i+1}-p_i}{\Delta x})^2 - ((q_i+\epsilon v_i)^2+p_i^2)^2 \\
&\quad - (\frac{q_{i+1}-q_i}{\Delta x})^2 + (\frac{p_{i+1}-p_i}{\Delta x})^2 + (q_i^2+p_i^2)^2] \\
&= \lim_{\epsilon\to 0}\frac{\Delta x}{2\epsilon}\sum_{i=0}^{N-1}\frac{2\epsilon(v_{i+1}-v_i)(q_{i+1}-q_i)}{(\Delta x)^2} - 2\epsilon v_i q_i + \mathcal{O}(\epsilon^2) \\
&= \Delta x\sum_{i=0}^{N-1}\frac{(v_{i+1}-v_i)(q_{i+1}-q_i)}{(\Delta x)^2} - q_i v_i.
\end{aligned}$$

By the periodic boundary conditions, we have

$$\sum_{i=0}^{N-1} v_{i+1}(q_{i+1}-q_i)\Delta x = \sum_{i=0}^{N-1} v_i(q_i - q_{i-1})\Delta x.$$

Therefore, we find

$$\langle \frac{\delta H}{\delta q_i}, v\rangle = \Delta x\sum_{i=0}^{N-1}\frac{v_i(q_i-q_{i-1}) - v_i(q_{i+1}-q_i)}{(\Delta x)^2} - q_i v_i = \Delta x\sum_{i=0}^{N-1} v_i\frac{-q_{i+1}+2q_i-q_{i-1}}{(\Delta x)^2} - q_i v_i.$$

from which we conclude $\frac{\delta H}{\delta q_i} = -\frac{q_{i+1}-2q_i+q_{i-1}}{(\Delta x)^2} - q_i$, for $i = 0 \ldots N-1$. Due to the symmetry of H, we find $\frac{\delta H}{\delta p_i} = -\frac{p_{i+1}-2p_i+p_{i-1}}{(\Delta x)^2} - p_i$, for $i = 0 \ldots N-1$.

We have now found all ingredients for the Hamiltonian spatial discretisation of the NLS equation. Since $\mathcal{J} = J$, we have:

$$\begin{aligned}
\dot{q}_i &= \frac{\delta H}{\delta p_i} = -\frac{p_{i+1}-2p_i+p_{i-1}}{(\Delta x)^2} - p_i. \\
\dot{p}_i &= -\frac{\delta H}{\delta q_i} = \frac{q_{i+1}-2q_i+q_{i-1}}{(\Delta x)^2} + q_i.
\end{aligned}$$

We want to know whether the discrete counterparts H, M and N of $\mathcal{H}$, $\mathcal{M}$ and $\mathcal{N}$ are conserved.

The discrete counterparts of $\mathcal{H}$ are conserved quantities: we have

$$\frac{\partial}{\partial t}H = \frac{\delta H}{\delta q}\dot{q} + \frac{\delta H}{\delta p}\dot{p} = -\dot{p}\dot{q} + \dot{q}\dot{p} = 0.$$

For N as the discrete counterpart of $\mathcal{N}$, we have

$$N = \sum_{i=0}^{N-1} |\psi_i|^2 \Delta x = \sum_{i=0}^{N-1} (p_i^2 + q_i^2)\Delta x$$

Note that N has two meanings now. However, from the context it's clear which one is which. The discrete counterpart of $\mathcal{N}$ is conserved, as we will show now. We have

$$\begin{aligned}
\frac{\partial}{\partial t}N &= 2\Delta x \sum_{i=0}^{N-1} p_i\dot{p}_i + q\dot{q}_i = 2\Delta x \sum_{i=0}^{N-1} p_i\left(\frac{q_{i+1} - 2q_i + q_{i-1}}{(\Delta x)^2} + q_i\right) - q_i\left(\frac{p_{i+1} - 2p_i + p_{i-1}}{(\Delta x)^2} + p_i\right),\\
&= 2\Delta x \sum_{i=0}^{N-1} p_i\frac{q_{i+1} - 2q_i + q_{i-1}}{(\Delta x)^2} - q_i\frac{p_{i+1} - 2p_i + p_{i-1}}{(\Delta x)^2},\\
&= 2\Delta x \sum_{i=0}^{N-1} \frac{p_i(q_{i+1} + q_{i-1}) - q_i(p_{i+1} + p_{i-1})}{(\Delta x)^2}.
\end{aligned}$$

For this sum, we have

$$\begin{aligned}
\sum_{i=0}^{N-1} p_iq_{i+1} + p_iq_{i-1} - q_ip_{i+1} - q_ip_{i-1} &= p_0q_1 + p_0q_{-1} - q_0p_1 - q_0p_{-1} + p_1q_2 + p_1q_0 - q_1p_2 - q_1p_0 + \dots + p_{N-2}q_{N-1}\\
&\quad + p_{N-2}q_{N-1} - q_{N-2}p_{N-1} - q_{N-2}p_{N-3} + p_{N-1}q_N + p_{N-1}q_{N-2} - q_{N-1}p_N - q_{N-1}p_{N-2}\\
&= p_0q_{-1} - q_0p_{-1} + p_{N-1}q_N - q_{N-1}p_N\\
&= p_Nq_{N-1} - q_Np_{N-1} + p_{N-1}q_N - q_{N-1}p_N = 0,
\end{aligned}$$

where the last line follows from the periodicity of ψ, i.e. we identify p_0 with p_N and q_0 with q_N. This also gives $p_{-1} = p_{N-1}$ and $q_{-1} = q_{N-2}$. We conclude that $\frac{\partial}{\partial t}N = 0$ and therefore N is a conserved quantity.

Finally, the quantity M as the discrete counterpart of $\mathcal{M}$ is given by:

$$\begin{aligned}
M &= \sum_{i=0}^{N-1} \psi_i(\psi_x)_i\Delta x = \Delta x \sum_{i=0}^{N-1} (q_i - ip_i)\left[\frac{q_{i+1} - q_i}{\Delta x} + i\frac{p_{i+1} - p_i}{\Delta x}\right].\\
&= \Delta x \sum_{i=0}^{N-1} \frac{q_i(q_{i+1} - q_i) + iq_i(p_{i+1} - p_i) - ip_i(q_{i+1} - q_i) + p_i(p_{i+1} - p_i)}{\Delta x}.\\
&= \Delta x \sum_{i=0}^{N-1} \frac{p_ip_{i+1} + q_iq_{i+1} + ip_{i+1}q_i - ip_iq_{i+1} - (p_i^2 + q_i^2)}{\Delta x}.
\end{aligned}$$

Then, we have

$$\frac{\partial}{\partial t}M = \Delta x \sum_{i=0}^{N-1} \frac{\dot{p}_ip_{i+1} + p_i\dot{p}_{i+1}\dot{q}_iq_{i+1} + q_i\dot{q}_{i+1} + i\dot{p}_{i+1}q_i + ip_{i+1}\dot{q}_i - i\dot{p}_iq_{i+1} - ip\dot{q}_{i+1} - 2p_i\dot{p}_i - 2q_i\dot{q}_i}{\Delta x}.$$

However, this sum is not equal to 0, since there are no terms that cancel by writing out the sum as we did for N. Therefore, M is not a conserved quantity.

(d)

Implicit midpoint rule

The implicit midpoint rule is a Runge Kutta method, which is of the form

$$F_i = f(y_n + \Delta t \sum_{j=1}^{s} a_{ij} F_j), i = 1, ..., s.$$

$$y_{n+1} = y_n + \Delta t \sum_{i=1}^{s} b_i F_i.$$

for $s = 1$, $a_{11} = \frac{1}{2}$ and $b = 1$. Indeed, this gives

$$y_{n+1} = y_n + \Delta t F_1, \text{ so } F_1 = \frac{y_{n+1} - y_n}{\Delta t},$$

$$F_1 = f(y_n + \Delta t \frac{1}{2} F_1) = f(y_n + \frac{1}{2}\Delta t(\frac{y_{n+1} - y_n}{\Delta t})).$$

Combining these two equations gives $\frac{y_{n+1}-y_n}{\Delta t} = f(\frac{y_{n+1}+y_n}{2})$, which is exactly the Implicit Midpoint Rule.

Firstly, we know that M is not a preserved quantity, so it's not a first integral. We know that both H and N are quadratic first integrals. For Runge-Kutta methods, the quadratic first integrals are preserved when the coefficients satisfy $b_i b_j - b_i a_{ij} - b_j a_{ji} = 0$ for $i, j = 1, ..., s$. For both H and N, we have

$$b_i b_j - b_i a_{ij} - b_j a_{ji} = 1 - \frac{1}{2} - \frac{1}{2} = 0$$

This means that the Implicit Midpoint Rule conserves arbitrary quadratic first integrals, which means that in our case, H and N are preserved.

We know that the Implicit Midpoint Rule is a symplectic method, since is a Runge Kutta method. Then, by backward error analysis we know that the modified equation, to which our approximation is a better solution than the original PDE, is again a Hamiltonian system. The perturbed Hamiltonian function is conserved by the modified equation, but not by the original PDE. Therefore, we expect none of the discrete integrals to be preserved to machine precision.