MC

$$\langle O(q) \rangle = \int O(q)\, \rho(q)\, d^{3N}q$$

$\rho(q)$: DISTRIBUTION NTV, NPT, GC

MD $O(q(t))$

$$\langle O(t) \rangle = \frac{1}{\tau} \int_0^{\tau} O(t)\, dt$$

TIME AVERAGE

MD MICROCANONICAL ENSEMBLE

HAMILTONIAN EQUATION

ISOLATED

NVE

$$\begin{cases} \dot{q}_i = \dfrac{\partial \mathcal{H}}{\partial p_i} \\ \dot{p}_i = -\dfrac{\partial \mathcal{H}}{\partial q_i} \end{cases} \qquad i = 1 \dots N$$

$\frac{\partial \mathcal{H}}{\partial t} = 0$ $\mathcal{H}$ DOES NOT DEPEND EXPLICITLY ON TIME

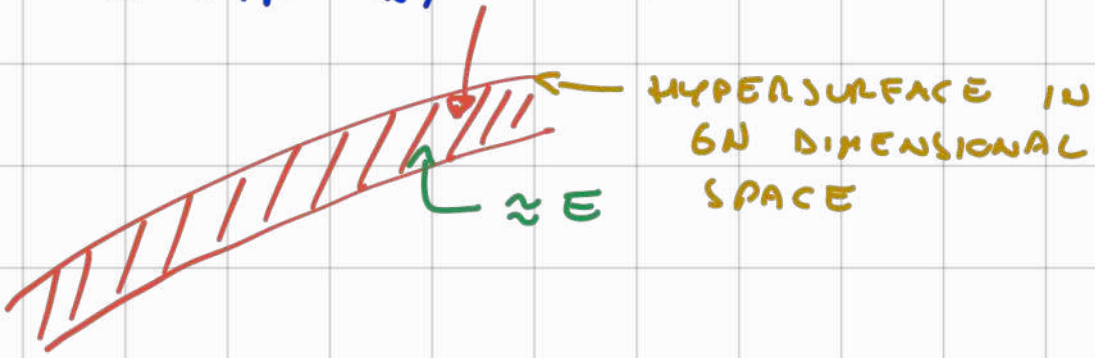
$$\mathcal{H}(q,p) = K + V = \sum_i^N \frac{\vec{p}_i^{\,2}}{2m} + V(\vec{q}_1 \dots \vec{q}_N)$$

$$\frac{d\mathcal{H}}{dt} = \sum_i \frac{\partial \mathcal{H}}{\partial \vec{q}_i} \dot{\vec{q}}_i + \frac{\partial \mathcal{H}}{\partial \vec{p}_i} \dot{\vec{p}}_i =$$

$$= \sum_i \frac{\partial \mathcal{H}}{\partial \vec{q}_i} \frac{\partial \mathcal{H}}{\partial \vec{p}_i} - \frac{\partial \mathcal{H}}{\partial \vec{p}_i} \frac{\partial \mathcal{H}}{\partial \vec{q}_i} = 0$$

ENERGY IS CONSERVED

$$\mathcal{H}(\vec{q}_1 \dots \vec{q}_N, \vec{p}_1 \dots \vec{p}_N) \approx E$$



$$\vec{P} = \sum_i \vec{p}_i$$

TOTAL MOMENTUM IS ALSO CONSERVED

$$\vec{L} = \sum_i \vec{r}_i \times \vec{p}_i$$

TOTAL ANGULAR MOMENTUM IS NOT CONSERVED IF WE RESTRICT TO SIMULATION BOX CENTERED AT ORIGIN

LAGRANGIAN FORMULATION

$$\mathcal{L} = K - V = \mathcal{L}(\vec{q}_1 \dots \vec{q}_N, \dot{\vec{q}}_1 \dots \dot{\vec{q}}_N)$$

$$\frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{\vec{q}}_i}\right) - \frac{\partial \mathcal{L}}{\partial \vec{q}_i} = 0 \Rightarrow \vec{F}_i = m_i \vec{a}_i$$

$$\ddot{\vec{q}}_i = \frac{\vec{F}_i}{m_i} \qquad i = 1 \dots N$$

LIOUVILLE'S THEOREM

HYDRODYNAMICS :

$\vec{v}(x)$ $\qquad \vec{J} = \rho \vec{v}$

$$\nabla \cdot \vec{J} + \frac{\partial \rho}{\partial t} = 0$$ CONTINUITY EQUATION

NOTE THAT

$$\nabla \cdot \vec{J} + \frac{\partial \rho}{\partial t} = \frac{\partial \rho}{\partial \vec{x}} \cdot \vec{v} + \rho \nabla \cdot \vec{v} + \frac{\partial \rho}{\partial t} =$$

IF WE DEFINE

$$\frac{D\rho}{Dt} \equiv \frac{\partial \rho}{\partial \vec{x}} \cdot \vec{v} + \frac{\partial \rho}{\partial t}$$ MATERIAL DERIVATIVE

$$\nabla \cdot \vec{J} + \frac{\partial \rho}{\partial t} = \frac{D\rho}{Dt} + \rho \nabla \cdot \vec{v} = 0$$

HENCE IF THE FLUID IS INCOMPRESSIBLE

$$\frac{D\rho}{Dt} = 0$$ WHICH IMPLIES

$$\frac{D\rho}{Dt} + \rho \nabla \cdot \vec{v} = \rho \nabla \cdot \vec{v} = 0 \Rightarrow \nabla \cdot \vec{v} = 0$$

AND ALSO THE OTHER WAY AROUND, I.E.

IF $\nabla \cdot \vec{v} = 0 \Rightarrow \frac{D\rho}{Dt} = 0$ I.E. THE FLUID IS INCOMPRESSIBLE

MAKING AN ANALOGY WITH HYDRODYNAMICS WE HAVE

$$\vec{v} = (\vec{q}_1 \dots \vec{q}_N, \vec{p}_1 \dots \vec{p}_N)$$

HENCE IF $\nabla \cdot \vec{v} = \sum_i^N \frac{\partial \dot{\vec{q}}_i}{\partial \vec{q}_i} + \sum_i^N \frac{\partial \dot{\vec{p}}_i}{\partial \vec{p}_i}$

BUT FOR AN HAMILTONIAN SYSTEM

$$\nabla \cdot \vec{v} = \sum_{i=1}^N \frac{\partial \dot{\vec{q}}}{\partial \vec{q}_i \partial \vec{p}_i} - \frac{\partial \dot{\vec{p}}}{\partial \vec{p}_i \partial \vec{q}_i} = 0$$

$K = \nabla \cdot \vec{v}$ IS CALLED COMPRESSIBILITY

WHICH IS THE LIOUVILLE'S THEOREM.

THIS IMPLIES THAT VOLUMES IN PHASE SPACE ARE CONSERVED WHEN THEY EVOLVE ACCORDING TO HAMILTONIAN EQUATIONS OF MOTION (SINCE ρ IS CONSTANT)

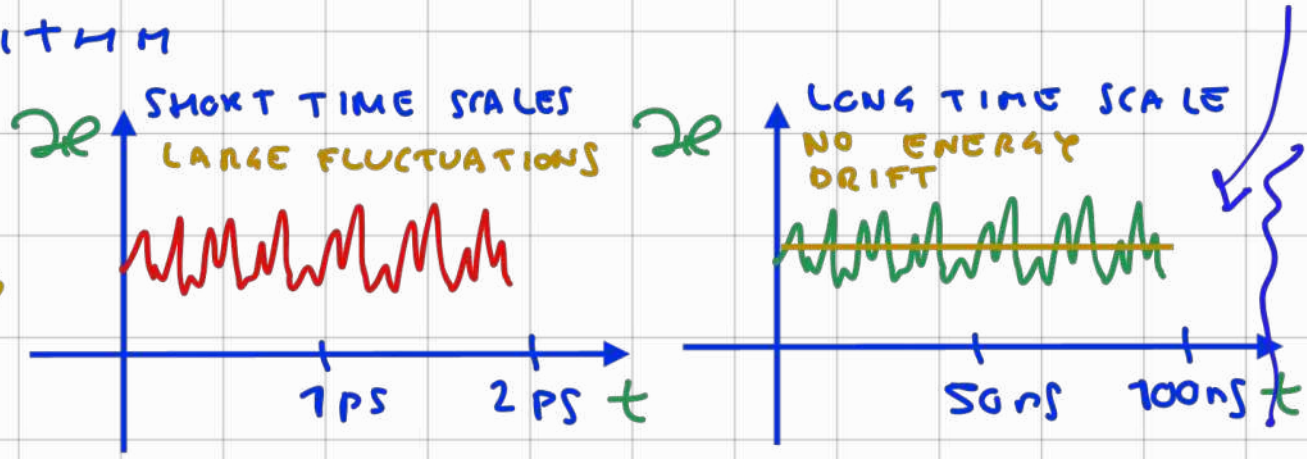
NUMERICAL INTEGRATION

WE WANT TO USE FINITE DIFFERENCE METHODS

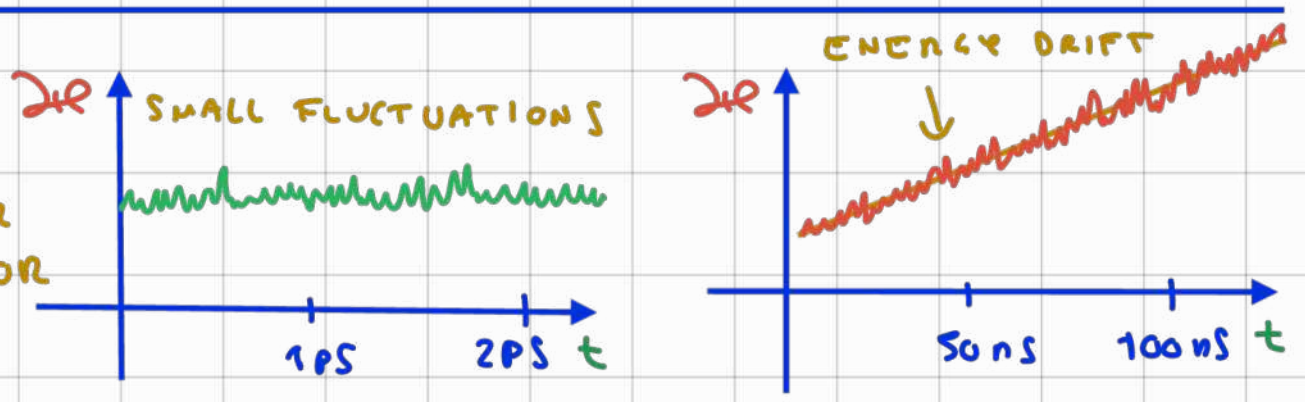
$$\vec{v}_i(t + \Delta t) = \vec{v}_i(t) + \vec{a}_i \Delta t + O(\Delta t^2)$$

THERE ARE TWO GENERAL ASPECTS TO TAKE INTO ACCOUNT FOR AN ALGORITHM

- VERLET
- VELOCITY VERLET
- LEAP-FROG



- GEAR PREDICTOR CORRECTOR



ENERGY DRIFT IS MORE IMPORTANT FOR HAVING ACCURATE TIME AVERAGES (IF ENERGY CHANGES IS LIKE HEATING UP OR COOLING DOWN THE SYSTEM)

VERLET, VELOCITY VERLET AND LEAP-FROG GUARANTEE A NEGLIGIBLE ENERGY DRIFT

VERLET ALGORITHM

① $\vec{r}_i(t+\Delta t) = \vec{r}_i(t) + \Delta t\, \vec{v}_i(t) + \frac{\Delta t^2}{2}\vec{a}_i(t) + O(\Delta t^3)$

② $\vec{r}_i(t-\Delta t) = \vec{r}_i(t) - \Delta t\, \vec{v}_i(t) + \frac{\Delta t^2}{2}\vec{a}_i(t) + O(\Delta t^3)$

IF WE SUM ① AND ② WE HAVE

$$\vec{r}_i(t+\Delta t) + \vec{r}_i(t-\Delta t) = 2\vec{r}_i(t) + \Delta t^2 \vec{a}_i(t) + \mathcal{O}(\Delta t^4)$$

$$\vec{r}_i(t+\Delta t) = 2\vec{r}_i(t) - \vec{r}_i(t-\Delta t) + \Delta t^2 \vec{a}_i(t) + \mathcal{O}(\Delta t^4)$$

$\vec{a}_i = \frac{\vec{F}_i}{m_i}$ ← TOTAL FORCE ACTING ON PARTICLE i

$\vec{F}_i = \vec{F}_i(\vec{r}_1 \dots \vec{r}_N)$

WITH

$$\vec{F}_e = -\frac{\partial}{\partial \vec{r}_e}\left(\sum_{i<j} v_2(|\vec{r}_i - \vec{r}_j|)\right)$$

INSTEAD IF WE SUBTRACT ① AND ② :

$$\vec{v}_i(t) = \frac{\vec{r}_i(t+\Delta t) - \vec{r}_i(t-\Delta t)}{2\Delta t} + \mathcal{O}(\Delta t^2)$$

THUS HAVING THE VELOCITY AT TIME t AND THE VERLET ALGORITHM READS :

$$\vec{r}_i(t+\Delta t) = 2\vec{r}_i(t) - \vec{r}_i(t-\Delta t) + \Delta t^2 \vec{a}_i(t) \quad \text{(V1)}$$

$$\vec{v}_i(t) = \frac{\vec{r}_i(t+\Delta t) - \vec{r}_i(t-\Delta t)}{2\Delta t} \quad \text{(V2)}$$

LEAP-FROG

$$\vec{r}_i(t+\Delta t) = \vec{r}_i(t) + \Delta t\, \vec{v}_i(t) + \frac{\Delta t^2}{2}\vec{a}_i(t) + \mathcal{O}(\Delta t^3)$$

$$\Delta t\, \vec{v}_i\left(t+\frac{\Delta t}{2}\right) = \Delta t\, \vec{v}_i(t) + \frac{\Delta t^2}{2}\vec{a}_i(t) + \mathcal{O}(\Delta t^3)$$

HENCE

FIRST EQUATION OF LEAP-FROG

$$\vec{r}_i(t+\Delta t) = \vec{r}_i(t) + \Delta t\, \vec{v}_i\left(t+\frac{\Delta t}{2}\right) + \mathcal{O}(\Delta t^3)$$

① $$\vec{v}_i\left(t+\frac{\Delta t}{2}\right) = \vec{v}_i(t) + \frac{\Delta t}{2}\vec{a}_i(t) + \mathcal{O}(\Delta t^2)$$

② $$\vec{v}_i\left(t-\frac{\Delta t}{2}\right) = \vec{v}_i(t) - \frac{\Delta t}{2}\vec{a}_i(t) + \mathcal{O}(\Delta t^2)$$

① − ②

$$\vec{v}_i\left(t+\frac{\Delta t}{2}\right) - \vec{v}_i\left(t-\frac{\Delta t}{2}\right) = \Delta t\, \vec{a}_i(t) + \mathcal{O}(\Delta t^3)$$

$$\vec{v}_i\left(t+\frac{\Delta t}{2}\right) = \vec{v}_i\left(t-\frac{\Delta t}{2}\right) + \Delta t\, \vec{a}_i(t) + \mathcal{O}(\Delta t^3)$$

↑ SECOND EQUATION OF LEAP-FROG

SO THAT THE LEAP-FROG ALGORITHM IS:

$$\vec{r}_i(t+\Delta t) = \vec{r}_i(t) + \Delta t\, \vec{v}_i\left(t+\frac{\Delta t}{2}\right) \qquad \text{(LF1)}$$

$$\vec{v}_i\left(t+\frac{\Delta t}{2}\right) = \vec{v}_i\left(t-\frac{\Delta t}{2}\right) + \Delta t\, \vec{a}_i(t) \qquad \text{(LF2)}$$

VELOCITY VERLET

① $\vec{r}_i(t+\Delta t) = \vec{r}_i(t) + \Delta t\, \vec{v}_i(t) + \frac{\Delta t^2}{2}\vec{a}_i(t) +$
$+ \frac{\Delta t^3}{6}\dot{\vec{a}}_i(t) + \mathcal{O}(\Delta t^4)$

② $\vec{r}_i(t) = \vec{r}_i((t+\Delta t)-\Delta t) =$
$\vec{r}_i(t+\Delta t) - \Delta t\, \vec{v}_i(t+\Delta t) + \frac{\Delta t^2}{2}\vec{a}_i(t+\Delta t) +$
$- \frac{\Delta t^3}{6}\dot{\vec{a}}_i(t+\Delta t) + \mathcal{O}(\Delta t^4) =$
$\vec{r}_i(t+\Delta t) - \Delta t\, \vec{v}_i(t+\Delta t) + \frac{\Delta t^2}{2}\vec{a}_i(t+\Delta t) +$
$- \frac{\Delta t^3}{6}\dot{\vec{a}}_i(t) + \mathcal{O}(\Delta t^4)$

① + ②:

$\vec{r}_i(t+\Delta t) + \vec{r}_i(t) =$
$\vec{r}_i(t+\Delta t) + \vec{r}_i(t) + \Delta t\, \vec{v}_i(t) +$
$- \Delta t\, \vec{v}_i(t+\Delta t) + \frac{\Delta t^2}{2}\left(\vec{a}_i(t) + \vec{a}_i(t+\Delta t)\right) +$
$+ \frac{\Delta t^3}{6}\dot{\vec{a}}_i(t) - \frac{\Delta t^3}{6}\dot{\vec{a}}_i(t) + \mathcal{O}(\Delta t^4)$

SECOND EQUATION

$$\vec{v}_i(t+\Delta t) = \vec{v}_i(t) + \frac{\Delta t}{2}\left(\vec{a}_i(t) + \vec{a}_i(t+\Delta t)\right) + \\ + \mathcal{O}(\Delta t^3)$$

FROM (1) BY CONSIDERING TERMS UP TO $\mathcal{O}(\Delta t^2)$:

$$\vec{r}_i(t+\Delta t) = \vec{r}_i(t) + \Delta t\,\vec{v}_i(t) + \frac{\Delta t^2}{2}\vec{a}_i(t) + \mathcal{O}(\Delta t^3)$$

FIRST EQUATION OF VELOCITY VERLET

HENCE VELOCITY VERLET ALGORITHM IS:

$$\vec{r}_i(t+\Delta t) = \vec{r}_i(t) + \Delta t\,\vec{v}_i(t) + \frac{\Delta t^2}{2}\vec{a}_i(t) \qquad (VV1)$$

$$\vec{v}_i(t+\Delta t) = \vec{v}_i(t) + \frac{\Delta t}{2}\left(\vec{a}_i(t) + \vec{a}_i(t+\Delta t)\right) \qquad (VV2)$$

THESE THREE ALGORITHMS ARE ALGEBRICALLY EQUIVALENT

INDEED THEY ARE ALL DERIVED FROM A TAYLOR EXPANSION OF $\vec{r}_i(t+\Delta t)$ UP TO SECOND ORDER

VERLET IS EQUIVALENT TO VELOCITY VERLET

FROM (V1):

$$\vec{r}_i(t+\Delta t) = 2\vec{r}_i(t) - \vec{r}_i(t-\Delta t) + \Delta t^2\,\vec{a}_i(t)$$

$$\vec{r}_i(t+\Delta t) = 2\vec{r}_i(t) - \vec{r}_i(t+\Delta t) + \vec{r}_i(t+\Delta t) - \vec{r}_i(t-\Delta t) + \\ + \Delta t^2\,\vec{a}_i(t)$$

BY USING (V2):

$$2\vec{r}_i(t+\Delta t) = 2\vec{r}_i(t) + 2\Delta t\,\vec{v}_i(t) + \Delta t^2\,\vec{a}_i(t)$$

$$\vec{r}_i(t+\Delta t) = \vec{r}_i(t) + \Delta t\,\vec{v}_i(t) + \frac{\Delta t^2}{2}\vec{a}_i(t)$$

WHICH IS (VV1)

CONCERNING (VV2) WE NEED TO PROVE THAT

$$\vec{v}_i(t+\Delta t) - \vec{v}_i(t) = \frac{\Delta t}{2}\left(\vec{a}_i(t) + \vec{a}_i(t+\Delta t)\right)$$

AND THIS CAN BE DONE BY USING EQ.(V2), I.E.

$$\vec{v}_i(t+\Delta t) - \vec{v}_i(t) =$$

$$\frac{\vec{r}_i(t+2\Delta t) - \vec{r}_i(t)}{2\Delta t} - \frac{\vec{r}_i(t+\Delta t) - \vec{r}_i(t-\Delta t)}{2\Delta t}$$

AND NOW WE CAN USE EQ. (V1) FOR BOTH $\vec{r}_i(t+2\Delta t)$ AND $\vec{r}_i(t-\Delta t)$ TO HAVE

$$2\vec{r}_i(t+\Delta t) - \vec{r}_i(t) - \vec{r}_i(t) + \Delta t^2 \vec{a}_i(t+\Delta t) +$$

$$- \vec{r}_i(t+\Delta t) + 2\vec{r}_i(t) - \vec{r}_i(t+\Delta t) + \Delta t^2 \vec{a}_i(t) =$$

$$= \Delta t^2 \left(\vec{a}_i(t) + \vec{a}_i(t+\Delta t)\right)$$

SO THAT

(*) FROM (V1): $\vec{r}_i(t-\Delta t) = 2\vec{r}_i(t) - \vec{r}_i(t+\Delta t) + \Delta t^2 \vec{a}_i(t)$

$$\vec{v}_i(t+\Delta t) - \vec{v}_i(t) = \frac{\Delta t}{2}\left(\vec{a}_i(t) + \vec{a}_i(t+\Delta t)\right)$$

WHICH IS (VV2)

LEAP-FROG IS EQUIVALENT TO VELOCITY-VERL.

WE WANT TO SHOW FIRST THAT

$$\vec{v}_i(t+\Delta t) - \vec{v}_i(t) = \frac{\Delta t}{2}\left(\vec{a}_i(t) + a_i(t+\Delta t)\right)$$

BUT FROM EQ. (LF2) BY ADVANCING BY HALF STEP

$$\vec{v}_i(t+\Delta t) = \vec{v}_i\left(t+\frac{\Delta t}{2}\right) + \frac{\Delta t}{2}\vec{a}_i(t+\Delta t) \quad (1)$$

SIMILARLY BY GOING BACK HALF TIME FROM $t+\frac{\Delta t}{2}$

$$\vec{v}_i(t) = \vec{v}_i\left(t+\frac{\Delta t}{2}\right) - \frac{\Delta t}{2}\vec{a}_i(t) \text{ I.E.}$$

$$\vec{v}_i(t+\Delta t/2) = \vec{v}_i(t) + \frac{\Delta t}{2}\vec{a}_i(t) \qquad (2)$$

HENCE IF WE SUM (1) AND (2):

$$\vec{v}_i(t+\Delta t) = \vec{v}_i(t) + \frac{\Delta t}{2}\left(\vec{a}_i(t) + \vec{a}_i(t+\Delta t)\right)$$

WHICH IS EQ. (VV2)

CONCERNING EQ.(VV1) WE NOTE THAT EQ.(LF1) IS:

$$\vec{r}_i(t+\Delta t) = \vec{r}_i(t) + \Delta t\, \vec{v}_i\left(t + \frac{\Delta t}{2}\right)$$

BUT FROM EQ.(2):

$$\vec{r}_i(t+\Delta t) = \vec{r}_i(t) + \Delta t\, \vec{v}_i(t) + \frac{\Delta t^2}{2}\vec{a}_i(t)$$

WHICH IS EQ. (VV1)

ENERGY CONSERVATION

$$\mathcal{H}(t) = \sum_i \frac{1}{2} m \vec{v}_i^2(t) + V(\vec{r}_1(t) .. \vec{r}_N(t))$$

WHERE $\{\vec{r}_i(t), \vec{v}_i(t)\}_i$ IS AN EXACT SOLUTION

IF FROM A FD ALGORITHM WE OBTAIN $\vec{r}_i^{FD}(\Delta t)$ AND $\vec{v}_i^{FD}(\Delta t)$ AS FOLLOWS:

$$\vec{r}_i^{FD}(\Delta t) = \vec{r}_i(\Delta t) + \mathcal{O}(\Delta t^3) \qquad (2)$$

(EXACT SOLUTION)

$$\vec{v}_i^{FD}(\Delta t) = \vec{v}_i(\Delta t) + \mathcal{O}(\Delta t^3) \qquad (3)$$

IF $\mathcal{H}^{FD}(\Delta t) \equiv \mathcal{H}(\vec{r}_1^{FD}(\Delta t) .. \vec{r}_N^{FD}(\Delta t), \vec{v}_1^{FD}(\Delta t) .. \vec{v}_N^{FD}(\Delta t))$

BY USING EQS. (2) AND (3) ONE HAS

$$\mathcal{H}^{FD}(\Delta t) = \mathcal{H}(\vec{r}_1(\Delta t) + \mathcal{O}(\Delta t^3) \ldots \vec{v}_N(\Delta t) + \mathcal{O}(\Delta t^3)) =$$

AND AFTER n STEPS:

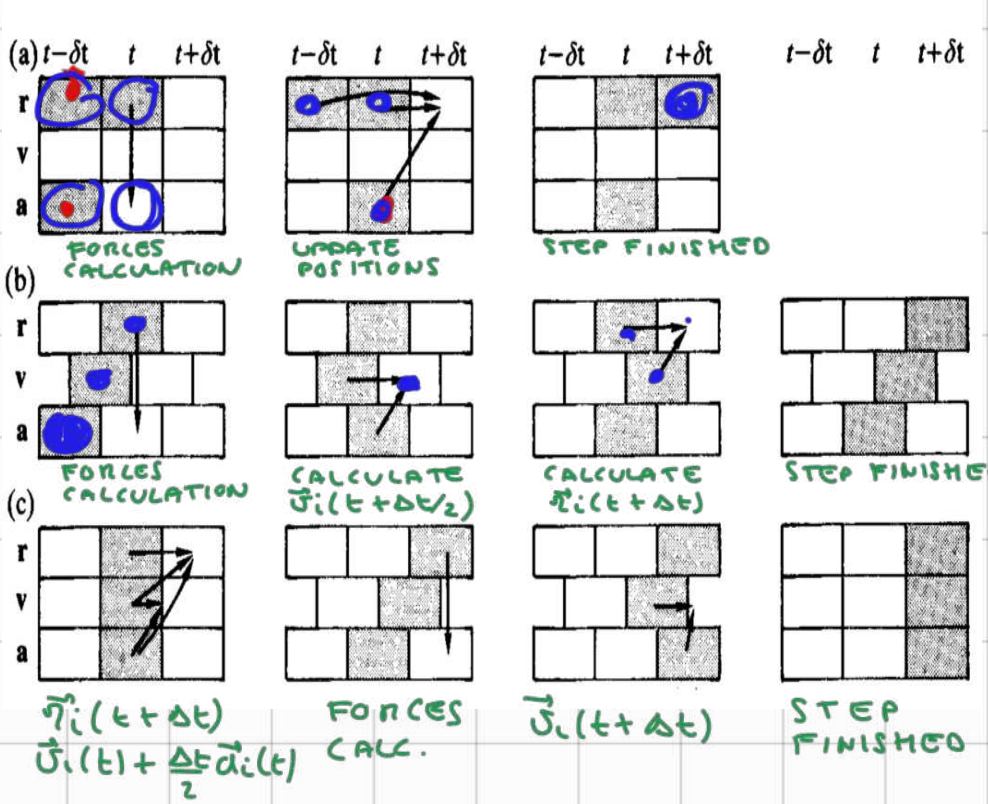
$$\mathcal{H}^{FD}(n\Delta t) = \mathcal{H}(\vec{r}_1(n\Delta t) + n\mathcal{O}(\Delta t^3) .. \vec{v}_N(n\Delta t) + n\mathcal{O}(\Delta t^3)) \approx$$

$\simeq \mathcal{H}(\vec{r}_1(n\Delta t)\ldots\vec{p}_N(n\Delta t)) + \underbrace{n\,\mathcal{O}(\Delta t^3)}_{\Delta\mathcal{H}}$

NOTE THAT THIS IS CORRECT ONLY IF $n\,\mathcal{O}(\Delta t^3) \ll 1$
I.E. FOR SHORT TIMES (SEE BELOW)
THIS IMPLIES THAT NOT NECESSARILY FLUCTUATIONS OF ENERGY INCREASES WITH TIME.
INDEED WE WILL SHOW BY THE SHADOW HAMILTONIAN THAT THEY ARE EXACTLY $\mathcal{O}(\Delta t^2)$
HENCE

$$\Delta\mathcal{H} = n\,\mathcal{O}(\Delta t^3) = n\Delta t\,\mathcal{O}(\Delta t^2) = t\,\underbrace{\mathcal{O}(\Delta t^2)}$$

QUADRATIC IN Δt



VERLET

$$\vec{r}_i(t+\Delta t) = 2\vec{r}_i(t) - \vec{r}_i(t-\Delta t) + \Delta t^2\vec{a}_i(t)$$

LEAP-FROG

$$\vec{r}_i(t+\Delta t) = \vec{r}_i(t) + \Delta t\,\vec{p}_i(t+\tfrac{\Delta t}{2})$$
$$\vec{p}_i(t+\tfrac{\Delta t}{2}) = \vec{p}_i(t-\tfrac{\Delta t}{2}) + \Delta t\,\vec{a}_i(t)$$

VELOCITY-VERLET

$$\vec{r}_i(t+\Delta t) = \vec{r}_i(t) + \Delta t\,\vec{p}_i(t) + \frac{\Delta t^2}{2}\vec{a}_i(t)$$
$$\vec{p}_i(t+\Delta t) = \vec{p}_i(t) + \frac{\Delta t}{2}\left(\vec{a}_i(t) + \vec{a}_i(t+\Delta t)\right)$$

SIMPLECTIC CONDITION

$$\dot{\vec{q}}_i = \frac{\partial \mathcal{H}}{\partial \vec{p}_i}$$

$$\dot{\vec{p}}_i = -\frac{\partial \mathcal{H}}{\partial \vec{q}_i}$$

$$\vec{Q} \equiv (\vec{q}_1 \dots \vec{q}_N) \qquad \vec{P} \equiv (\vec{p}_1 \dots \vec{p}_N)$$

$$X \equiv \begin{pmatrix} \vec{Q} \\ \vec{P} \end{pmatrix}$$ COLUMN VECTOR

THEN WE CAN REWRITE HAMILTON EQS. AS FOLLOWS:

$$\dot{X} = J^t \left(\frac{\partial \mathcal{H}}{\partial X} \right)$$ ← TRANSPOSE

WITH

$$J = \begin{pmatrix} 0 & \mathbb{1} \\ -\mathbb{1} & 0 \end{pmatrix}$$

$\mathbb{1}$ = 3N x 3N IDENTITY

J = 6N x 6N MATRIX

$\frac{\partial}{\partial X}$ IS A ROW VECTOR

COORDINATE TRANSFORMATION

$$Y = Y(X)$$

IF THIS TRANSFORMATION IS CANONICAL FORM OF HAMILTON EQS. MUST BE UNCHANGED, I.E.

$$\dot{\psi} = J^{t}\left(\frac{\partial \mathcal{H}}{\partial \psi}\right)$$

BUT

$$\dot{\psi} = \frac{d}{dt}(\psi(x)) = \frac{\partial \psi}{\partial x}\,\dot{x}$$

$$\frac{\partial \psi}{\partial x} = \begin{pmatrix} \frac{\partial \psi_1}{\partial x_1} & \cdots & \frac{\partial \psi_1}{\partial x_N} \\ \vdots & & \\ \frac{\partial \psi_N}{\partial x_1} & \cdots & \frac{\partial \psi_N}{\partial x_N} \end{pmatrix}$$

JACOBIAN OF TRANSFORMATION

$$\dot{x} = J^{t}\left(\frac{\partial \mathcal{H}}{\partial x}\right)$$

HENCE

$$\dot{\psi} = \frac{\partial \psi}{\partial x}\, J^{t}\left(\frac{\partial \mathcal{H}}{\partial x}\right)$$

$$\frac{\partial \mathcal{H}}{\partial x} = \frac{\partial \mathcal{H}}{\partial \psi}\,\frac{\partial \psi}{\partial x}$$ (CHAIN RULE)

THEREFORE

$$\dot{\eta} = \frac{\partial \varphi}{\partial x} J^t \left(\frac{\partial \mathcal{H}_\varphi}{\partial \varphi} \frac{\partial \varphi}{\partial x} \right) =$$

$$= \frac{\partial \varphi}{\partial x} J^t \left(\frac{\partial \varphi}{\partial x} \right) {}^t \left(\frac{\partial \mathcal{H}_\varphi}{\partial \varphi} \right)$$

IF TRANSFORMATION IS CANONICAL:

$$\frac{\partial \varphi}{\partial x} J^t \left(\frac{\partial \varphi}{\partial x} \right) = J$$

IF $\frac{\partial \varphi}{\partial x} = M$

$$\boxed{M J {}^t M = J}$$ SIMPLECTIC CONDITION

IF THIS CONDITION HOLDS, INDEED

$$\dot{\eta} = J^t \left(\frac{\partial \mathcal{H}_\varphi}{\partial \varphi} \right)$$

LET'S CONSIDER THE MAPPING (TRANSFORMATION) INDUCED BY THE SOLUTION OF HAMILTON'S EQUATIONS, I.E.

$$\underset{\parallel}{X(t)} = \phi (t, \underset{\parallel}{X_0})$$
$$\eta \qquad\qquad\qquad\quad X$$

$$\eta = \varphi(x)$$

THIS MAPPING IS CANONICAL

PROOF (POINCARE' THEOREM)

$X(t) = \phi(t, X_0)$ TIME EVOLUTION ACCORDING TO HAMILTON EQS.

$X_0 \rightarrow X(t)$ MAPPING

$M(t) = \dfrac{\partial \phi(t, X_0)}{\partial X_0}$ JACOBIAN OF TRANSFORMATION

SYMPLECTIC CONDITION READS

$$M(t)\, J\, {}^tM(t) = J \qquad (C1)$$

AT $t=0$ THIS CONDITION IS FULFILLED, SINCE

$$M(0) = \left.\frac{\partial \phi(t, X_0)}{\partial X_0}\right|_{t=0} = \mathbb{1}$$

SO THAT (C1) REDUCES TO

$$J = J$$

HENCE, IF WE PROVE THAT :

$$\frac{d}{dt}\left(M(t)\, J\, {}^tM(t) \right) = 0 \qquad \forall t \qquad (P1)$$

THIS ENSURES THAT CONDITION (C1) IS FULFILLED $\forall t$

FIRST WE PROVE THAT CONDITION (C1) IS EQUIVALENT TO :

$${}^tM\, J\, M = J \qquad (C2)$$

INDEED

$$J = \begin{pmatrix} 0 & \mathbb{1} \\ -\mathbb{1} & 0 \end{pmatrix} \Rightarrow J^2 = \begin{pmatrix} -\mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{pmatrix} = -\mathbb{1}$$

AND

$$^tJ\,J = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & \mathbb{1} \end{pmatrix} = \mathbb{1}$$

$$M J\, {}^tM = J$$

$$M J\, \underbrace{{}^tM ({}^tM)^{-1}}_{\mathbb{1}} = J({}^tM)^{-1}$$

$$MJ = J({}^tM)^{-1} \qquad (3)$$

MOREOVER CONSIDER

$$\boxed{J(MJ)J} = J M J^2 = \boxed{-JM} \qquad (4)$$

BY USING (3) :

$$\boxed{J(MJ)J} = J(J({}^tM)^{-1})J =$$

$$\underbrace{JJ}_{-\mathbb{1}} ({}^tM)^{-1} J = \boxed{-({}^tM)^{-1} J} \qquad (5)$$

FROM (4) AND (5):

$$-JM = -({}^tM)^{-1} J$$

I.E.

$$^tM\,J\,M = {}^tM\cancel{({}^tM)^{-1}}\,\mathbb{1}\,J$$

$$\Downarrow$$

$$\boxed{{}^tM\,J\,M = J}$$

HENCE EQ. (P1) IS EQUIVALENT TO:

$$\frac{d}{dt}\left({}^t M(t)\, J\, M(t)\right) = 0$$

I.E.

$${}^t\dot{M}\, J\, M + {}^t M J \dot{M} = 0 \qquad (C6)$$

BUT

$$\dot{M} = \frac{d}{dt}[M(t)] = \frac{d}{dt}\left[\frac{\partial \phi(t,x_0)}{\partial x_0}\right] = \frac{\partial}{\partial x_0}\left[\dot{\phi}(t,x_0)\right]$$

SINCE $\phi(t,x_0)$ IS A SOLUTION OF HAMILTON'S EQUATIONS:

$$\dot{\phi}(t,x_0) = J\, {}^t\left(\frac{\partial \mathcal{H}}{\partial x}\right)_{x=\phi(t,x_0)}$$

REMEMBER THAT $x = (\vec{q}_1 \ldots \vec{q}_N, \vec{p}_1 \ldots \vec{p}_N)$

$$\frac{\partial}{\partial x_0}\left[\dot{\phi}(t,x_0)\right] = \frac{\partial}{\partial x_0}\left[J\, {}^t\left(\frac{\partial \mathcal{H}}{\partial x}\right)_{x=\phi(t,x_0)}\right] =$$

$$= J \left.\frac{\partial^2 \mathcal{H}}{\partial x\, \partial x}\right|_{x=\phi(t,x_0)} \frac{\partial \phi}{\partial x_0} = J\, H_{xx}\, M$$

$\frac{\partial \phi}{\partial x_0} = M$

${}^t\left(\frac{\partial \mathcal{H}}{\partial x}\right)$ IS A COLUMN VECTOR, HENCE $\frac{\partial}{\partial x}\left[{}^t\left(\frac{\partial \mathcal{H}}{\partial x}\right)\right]$ IS A MATRIX

WHERE

$$H_{xx} = \left.\frac{\partial^2 \mathcal{H}}{\partial x\, \partial x}\right|_{x=\phi(t,x_0)}$$

THEREFORE

$$\dot{M} = J\, H_{xx}\, M \qquad \text{AND} \qquad (C7)$$

$${}^t\dot{M} = {}^t M\, H_{xx}\, {}^t J \qquad (H_{xx} = {}^t H_{xx}) \qquad (C8)$$

CONSIDER EQ. ((6), I.E.

$$ {}^t\dot{M} J M + {}^t M J \dot{M} = 0 $$

WHICH BY USING EQS. ((7) AND ((8) BECOMES:

$$ \underbrace{{}^t M H_{xx}}_{-\mathbb{1}} \underbrace{{}^t J J}_{\mathbb{1}} M + {}^t M \underbrace{J J}_{-\mathbb{1}} H_{xx} M = $$

$$ = {}^t M H_{xx} M - {}^t M H_{xx} M = 0 $$

THUS PROVING THE POINCARÈ THEOREM

MAPPING INDUCED BY SOLUTION OF HAMILTON'S EQUATION'S IS CANONICAL

LIOUVILLE'S THEOREM (AGAIN)

IF $\phi(t, X_0)$ IS A SOLUTION OF HAMILTON'S EQUATIONS AND

AND $M = \dfrac{\partial \phi(t, X_0)}{\partial X_0}$ FROM POINCARÈ'S THEOREM IT FOLLOWS THAT:

$$ M J {}^t M = J $$

BUT

$$ \det(M J {}^t M) = \det(J) $$

$$ \det(M) \det(J) \det({}^t M) = \det(J) $$

SINCE $\det(J) = 1$ AND $\det({}^tM) = \det(M)$

$$(\det(M))^2 = 1$$

I.E.

$$|\det M| = 1$$

WHICH MEANS THAT VOLUMES OF PHASE SPACE ARE PRESERVED BY THE MAPPING INDUCED BY SOLUTION OF HAMILTON'S EQS. I.E. LIOUVILLE'S THEOREM



LIOUVILLE'S OPERATOR

BE $\phi(q,p)$ A FUNCTION OF (q,p)

$q = q(t) \quad p = p(t)$

SOLUTION OF HAMILTON'S EQUATIONS

$$\phi(t) = \phi(q(t), p(t))$$

HENCE

$$\dot{\phi} = \frac{\partial \phi}{\partial q}\dot{q} + \frac{\partial \phi}{\partial p}\dot{p} = \frac{\partial \phi}{\partial q}\frac{\partial \mathcal{H}}{\partial p} - \frac{\partial \phi}{\partial p}\frac{\partial \mathcal{H}}{\partial q}$$

IF WE ASSUME $\mathcal{H} = \frac{p^2}{2m} + V(q)$

$$= \frac{\partial \phi}{\partial q}\frac{p}{m} + \frac{\partial \phi}{\partial p} f = \underbrace{\left(\frac{p}{m}\frac{\partial}{\partial q} + F\frac{\partial}{\partial p}\right)}\phi(q,p)$$

OPERATOR WHICH ACTS ON FUNCTIONS OF q AND p

$$i\mathcal{L} \equiv \frac{p}{m}\frac{\partial}{\partial q} + f\frac{\partial}{\partial p}$$

LIOUVILLE'S OPERATOR

$$\dot{\phi} = i\mathcal{L}\,\phi(q,p)\Big|_{\substack{q=q(t)\\p=p(t)}}$$

FOR N PARTICLES WE HAVE

$$i\mathcal{L} = \sum_{i=1}^{N} \frac{\vec{p}_i}{m_i}\cdot\frac{\partial}{\partial \vec{q}_i} + \vec{f}_i\cdot\frac{\partial}{\partial \vec{p}_i} \qquad \begin{matrix}\vec{q}_1 \dots \vec{q}_N\\ \vec{p}_1 \dots \vec{p}_N\end{matrix}$$

SCALAR PRODUCT

LET'S CONSIDER THE OPERATOR

$$\mathbb{1} + i\mathcal{L}\Delta t$$

$\mathbb{1}$: IDENTITY OPERATOR

THEN IF $\Gamma(0) = \begin{pmatrix} q(0) \\ p(0) \end{pmatrix}$

$$(\mathbb{1} + i\mathcal{L}\Delta t)\,\Gamma(0) = (\mathbb{1} + i\mathcal{L}\Delta t)\begin{pmatrix} q(0) \\ p(0) \end{pmatrix} =$$

$$= \begin{pmatrix} (\mathbb{1} + i\mathcal{L}\Delta t)\,q \\ (\mathbb{1} + i\mathcal{L}\Delta t)\,p \end{pmatrix}\Bigg|_{\substack{q=q(0) \\ p=p(0)}} = \begin{pmatrix} q(0) + \Delta t\,\dfrac{p(0)}{m} \\ p(0) + \Delta t\, f(0) \end{pmatrix} =$$

$$= \begin{pmatrix} q(\Delta t) \\ p(\Delta t) \end{pmatrix} = \Gamma(\Delta t)$$

NOTE THAT

i.e. $\phi(q,p) = q$ IN THIS CASE

$$(\mathbb{1} + i\mathcal{L}\Delta t)\,q(0) = (\mathbb{1} + i\mathcal{L}\Delta t)\,q\,\Big|_{\substack{q=q(0) \\ p=p(0)}} =$$

$$= q(0) + \frac{p(0)}{m}\Delta t = q(\Delta t)$$

AND SIMILARLY

i.e. $\phi(q,p) = p$ IN THIS CASE

$$(\mathbb{1} + i\mathcal{L}\Delta t)\,p(0) = (\mathbb{1} + i\mathcal{L}\Delta t)\,p\,\Big|_{\substack{q=q(0) \\ p=p(0)}} =$$

$$= p(0) + f(0)\Delta t = p(\Delta t)$$

IN GENERAL SINCE

SINCE $i\mathcal{L}\,\phi(0) = \dot{\phi}(0)$

$$\phi(\Delta t) = \phi(0) + \dot{\phi}(0)\Delta t = (\mathbb{1} + i\mathcal{L}\Delta t)\,\phi(0)$$

LET'S CONSIDER n APPLICATION OF OPERATOR $\mathbb{1} + i\mathcal{L}\Delta t$ WITH $t = n\Delta t$ AND n LARGE:

$$\boxed{(\mathbb{1} + i\mathcal{L}\Delta t)^n\,\Gamma(0)} = \lim_{n\to+\infty}\left(n + i\mathcal{L}\frac{t}{n}\right)^n \Gamma(0) =$$

$$\boxed{= e^{i\mathcal{L}t}\,\Gamma(0) = \Gamma(t)}$$

$e^{i\mathcal{H}t}$ IS THE PROPAGATOR OR TIME EVOLUTION OPERATOR

ANALOGY WITH QUANTUM MECHANICS

$$|\psi, t\rangle = e^{-i\frac{\hat{H}t}{\hbar}} |\psi\rangle$$

WHERE $\hat{H}$ IS THE HERMITIAN HAMILTONIAN OPERATOR

AND $\hat{U} = e^{-i\frac{\hat{H}t}{\hbar}}$ IS THE UNITARY TIME EVOLUTION OPERATOR

INDEED SINCE $\hat{H}^+ = \hat{H}$

$$\left(e^{-i\frac{\hat{H}t}{\hbar}}\right)^+ = e^{i\frac{\hat{H}^+ t}{\hbar}} = e^{i\frac{\hat{H}t}{\hbar}} = \hat{U}^{-1}$$

I.E. $U^+ U = \hat{U}^{-1}\hat{U} = \mathbb{1}$

HENCE

$$\langle \psi, t | \psi, t \rangle = \langle \psi | \underbrace{e^{-i\frac{\hat{H}t}{\hbar}} e^{i\frac{\hat{H}t}{\hbar}}}_{\mathbb{1}} | \psi \rangle =$$

$$= \langle \psi | \psi \rangle$$

I.E. PROBABILITIES ARE CONSERVED

IF WE CONSIDER A GENERIC OPERATOR $\hat{\mathcal{O}}$ AND A COMPLETE SET ψ_e WE HAVE

$$\langle \psi_k | \hat{\mathcal{O}} | \psi_e \rangle = \hat{\mathcal{O}}_{ke}$$

E.G. IF WE CONSIDER EIGENSTATES OF POSITION OPERATOR

WE HAVE

$$\int |x><x| d^{3N}x = \mathbb{1}$$

HENCE

$$<\psi_k | \hat{\mathcal{O}} | \psi_\ell>$$

$$= \int <\psi_k | x><x| \hat{\mathcal{O}} |x'><x'|\psi_\ell> d^{3N}x\, d^{3N}x'$$

FOR EXAMPLE IF $\hat{\mathcal{O}} = \hat{p}$ ONE HAS

$$= \int \psi_k^*(x)\, \delta(x-x') \left(-i\hbar \frac{\partial}{\partial x}\right) \psi_\ell(x')\, d^{3N}x\, d^{3N}x' =$$

$$= \int \psi_k^*(x) \left(-i\hbar \frac{\partial}{\partial x}\right) \psi_\ell(x)\, d^{3N}x$$

IN OUR PRESENT CASE OF LIOUVILLIAN FORMALISM, IF $\{\phi_k(q,p)\}_k$ IS A COMPLETE SET, THEN:

$$(\mathcal{L})_{k\ell} = \int \phi_k^*(q,p)\, \mathcal{L}\, \phi_\ell(q,p)\, dq\, dp$$

MOREOVER IF $\mathcal{L}$ IS HERMITIAN $e^{i\mathcal{L}t}$ IS UNITARY AND

$$e^{i\mathcal{L}t}\phi(0) = \phi(t) = \phi_t(q,p) \quad \text{I.E.}$$

$$e^{i\mathcal{L}t}\,\phi(q,p) = \phi(q'(t,q,p), p'(t,q,p))$$

$$= \phi_t(q,p)$$

WHERE $e^{i\mathcal{L}t}\begin{pmatrix} q \\ p \end{pmatrix} = \begin{pmatrix} q' \\ p' \end{pmatrix}$

HENCE

$$\langle \phi_t \mid \phi_t \rangle = \int \phi_t^* \, \phi_t \, dq\,dp =$$

$U^{-1} = U^*$

$$\int \phi^*(0)\, e^{-i\mathcal{L}t}\, e^{i\mathcal{L}t}\, \phi(0)\, dq\,dp =$$

$$\int \phi^*(0)\, \phi(0)\, dq\,dp = \langle \phi_0 \mid \phi_0 \rangle$$

I.E. VOLUMES OF PHASE SPACE ARE CONSERVED, INDEED IF

$$\phi(q,p) = \begin{cases} 1 & (q,p) \in V \\ 0 & \text{OTHERWISE} \end{cases}$$

WHICH IS AGAIN THE LIOUVILLE'S THEOREM

LET'S SHOW THAT $\mathcal{L}$ IS HERMITIAN

$$\mathcal{H} = \frac{p}{2m} + V(q)$$

$\{\phi_k(q,p)\}_k$ COMPLETE SET SUCH THAT

$\phi_k(q,p) \to 0$ FOR LARGE q OR p

$$(\mathcal{L})_{ke} = \int \phi_k^* \, \mathcal{L} \, \phi_e \, dq\,dp \,.$$

$$i\mathcal{L} = \frac{p}{m}\frac{\partial}{\partial q} + f\frac{\partial}{\partial p}$$

$$\mathcal{L} = (-i)\left(\frac{p}{m}\frac{\partial}{\partial q} + f\frac{\partial}{\partial p}\right)$$

HENCE

$$(\mathcal{L}_{ke}) = (-i)\int \phi_k^*\left(\frac{p}{m}\frac{\partial}{\partial q} + f\frac{\partial}{\partial p}\right)\phi_e\, dq\, dp$$

BE $i\mathcal{L}_q \equiv \frac{p}{m}\frac{\partial}{\partial q}$ AND $i\mathcal{L}_p \equiv f\frac{\partial}{\partial p}$

IF WE PROVE THAT BOTH $\mathcal{L}_q$ AND $\mathcal{L}_p$ ARE HERMITIAN THEN $\mathcal{L}$ IS HERMITIAN

$\mathcal{L}_q$:

$$(\mathcal{L}_q)_{ke} = \int \phi_k^*\, \mathcal{L}_q\, \phi_e\, dq\, dp$$

$$(\mathcal{L}_q)^*_{ek} = \left(\int \phi_e^*\ \mathcal{L}_q\ \phi_k\, dq\, dp\right)^* =$$

$$= \left((-i)\int \phi_e^* \frac{p}{m}\frac{\partial}{\partial q}\phi_k\, dq\, dp\right)^* =$$

$$= i\left(\int \phi_e^* \frac{p}{m}\frac{\partial}{\partial q}\phi_k\, dq\, dp\right)^* =$$

INTEGRATING BY PARTS AND EXPLOITING THE FACT THAT $\phi_k(q,p) \to 0$ $(q,p) \to +\infty$

ONE HAS :

$$= -i \left(\int \frac{\partial}{\partial q} \left(\phi_e^* \frac{p}{m} \right) \phi_k \, dq \, dp \right)^* =$$

$$= -i \int \phi_k^* \frac{p}{m} \frac{\partial}{\partial q} \phi_e \, dq \, dp =$$

$$= (\mathcal{L}_q)_{ke}$$

I.E WE HAVE PROVED THAT

$(\mathcal{L}_q)^*_{ek} = (\mathcal{L}_q)_{ke}$ I.E.

$\mathcal{L}_q^+ = \mathcal{L}_q \Rightarrow \mathcal{L}_q$ IS HERMITIAN

$\mathcal{L}_p$:

$$(\mathcal{L}_p)^*_{ek} = \left((-i) \int \phi_e^* \, F \frac{\partial}{\partial p} \phi_k \, dq \, dp \right)^* =$$

INTEGRATING BY PARTS WITH $\phi_k(q,p) \to 0$ IF $(q,p) \to +\infty$

$$= -i \int \phi_k^* \frac{\partial}{\partial p} (f \phi_e) \, dq \, dp =$$

NOW IF $f = f(q)$ I.E. FORCES DO NOT DEPEND ON p ONE HAS:

$$= -i \int \phi_k^* \, f \frac{\partial}{\partial p} \phi_e \, dq \, dp = (\mathcal{L}_p)_{ke}$$

I.E. $(\mathcal{L}_p)^*_{ek} = (\mathcal{L}_p)_{ke}$

$$\mathcal{L}_p^+ = \mathcal{L}_p$$

AND $\mathcal{L}_p$ IS HERMITIAN

THUS $\mathcal{L}$ IS HERMITIAN AND

$e^{i\mathcal{L}t}$ IS UNITARY

NOTE THAT IF WE HAVE

$$\begin{cases} \dot{q} = \frac{p}{m} \\ \dot{p} = f + \alpha p \end{cases}$$

SINCE

$$i\mathcal{L}\underbrace{\begin{pmatrix} q \\ p \end{pmatrix}}_{\phi} = \underbrace{\begin{pmatrix} p/m \\ f + \alpha p \end{pmatrix}}_{\dot{\phi}}$$

WE HAVE

$$i\mathcal{L} = \frac{p}{m}\frac{\partial}{\partial q} + F\frac{\partial}{\partial p} + \alpha p \frac{\partial}{\partial p}$$

WHICH IS NOT HERMITIAN

BUILDING ALGORITHMS BY APPROXIMATING THE TIME EVOLUTION OPERATOR $e^{i\mathcal{L}t}$

WE WANT TO FIND A STRATEGY TO HAVE

$$\phi(\Delta t) = \phi_{FD}(\Delta t, x_0)$$

(x_0: INITIAL CONDITION)

WHERE THIS APPROXIMATE SOLUTION MUST PRESERVE SOME PROPERTIES OF EXACT SOLUTION

$$i\mathcal{L} = i\mathcal{L}_q + i\mathcal{L}_p$$

HENCE

$$e^{i\mathcal{L}\Delta t} = e^{i\mathcal{L}_q\Delta t + i\mathcal{L}_p\Delta t} = U_{Ex}(\Delta t)$$

A POSSIBLE APPROXIMATE SOLUTION BASED ON TROTTER'S THEOREM:

$$\tilde{U}(\Delta t) = e^{i\mathcal{L}_q\Delta t}\, e^{i\mathcal{L}_p\Delta t} + \mathcal{O}(\Delta t^n)$$

WHERE n HAS TO BE DETERMINED

BEFORE ESTIMATING n, LET'S SHOW THAT $\mathcal{L}_q$ AND $\mathcal{L}_p$ DO NOT COMMUTE

$$[\mathcal{Y}_1, \mathcal{L}_p] = \mathcal{L}_q \mathcal{L}_p - \mathcal{L}_p \mathcal{L}_q =$$

$$= -[i\mathcal{L}_q, i\mathcal{L}_p] \neq 0$$

BUT

$$i\mathcal{L}_q \, i\mathcal{L}_p \, \phi(q,p) = \frac{p}{m} \frac{\partial}{\partial q} \left(f(q) \frac{\partial}{\partial p} \phi(q,p) \right) =$$

$$= \frac{p}{m} \frac{\partial f(q)}{\partial q} \frac{\partial \phi(q,p)}{\partial p} + \frac{p}{m} f(q) \frac{\partial \phi(q,p)}{\partial q \partial p}$$

AND

$$i\mathcal{L}_p \, i\mathcal{L}_q \, \phi(q,p) = f(q) \frac{\partial}{\partial p} \left(\frac{p}{m} \frac{\partial}{\partial q} \phi(q,p) \right) =$$

$$= \frac{f(q)}{m} \frac{\partial \phi(q,p)}{\partial q} + \frac{p}{m} f(q) \frac{\partial \phi(q,p)}{\partial p \partial q}$$

$$(i\mathcal{L}_q \, i\mathcal{L}_p - i\mathcal{L}_p \, i\mathcal{L}_q) \, \phi(q,p) =$$

$$= \frac{p}{m} \frac{\partial f(q)}{\partial q} \frac{\partial \phi(q,p)}{\partial p} - \frac{f(q)}{m} \frac{\partial \phi(q,p)}{\partial q}$$

$$\neq 0$$

NOW LET'S EXPAND $U_{ex}(\Delta t)$ WE GET:

$$U_{ex}(\Delta t) = \mathbb{1} + i(\mathcal{L}_q + \mathcal{L}_p)\Delta t + \frac{1}{2}(i\mathcal{L}_q + i\mathcal{L}_p)^2 \Delta t^2 + \mathcal{O}(\Delta t^3) =$$

$$= \mathbb{1} + (i\mathcal{L}_q + i\mathcal{L}_p)\Delta t + \frac{1}{2}(i\mathcal{L}_q)^2 \Delta t^2 + \frac{1}{2}(i\mathcal{L}_p)^2 \Delta t^2 + \frac{1}{2} i\mathcal{L}_q \mathcal{L}_p \Delta t^2 + \frac{1}{2} i\mathcal{L}_p i\mathcal{L}_q \Delta t^2 +$$

$+ O(\Delta t^3)$

IF EXPAND $\tilde{U}(\Delta t)$, WE GET :

$$\tilde{U}(\Delta t) = [\mathbb{1} + i\mathcal{L}_q \Delta t + (i\mathcal{L}_q)^2 \frac{\Delta t^2}{2} + O(\Delta t^3)][\mathbb{1} + i\mathcal{L}_p \Delta t + (i\mathcal{L}_p)^2 \frac{\Delta t^2}{2} + O(\Delta t^3)] = \mathbb{1} + (i\mathcal{L}_q + i\mathcal{L}_p)\Delta t + (i\mathcal{L}_q)^2 \frac{\Delta t^2}{2} + (i\mathcal{L}_p)^2 \frac{\Delta t^2}{2} + i\mathcal{L}_q i\mathcal{L}_p \Delta t^2 + O(\Delta t^3)$$

THEN SINCE $\mathcal{L}_q$ AND $\mathcal{L}_p$ DOES NOT COMMUTE :

$$\tilde{U}(\Delta t) = U_{Ex}(\Delta t) + i\mathcal{L}_q i\mathcal{L}_p \frac{\Delta t^2}{2} - i\mathcal{L}_p i\mathcal{L}_q \frac{\Delta t^2}{2} + O(\Delta t^3) = U_{Ex}(\Delta t) + \underbrace{O(\Delta t^2)}_{\text{ERROR}}$$

THUS

$$e^{i\mathcal{L}\Delta t} \approx e^{i\mathcal{L}_q \Delta t} e^{i\mathcal{L}_p \Delta t} + O(\Delta t^2) \quad (1)$$

CONSIDER ALSO ANOTHER PROPRIETY OF HAMILTON EQUATION WHICH IS THE TIME REVERSIBILITY, I.E.

$$U_{Ex}(t) = e^{i\mathcal{L}t}$$

$$U_{Ex}(-t) = e^{-i\mathcal{L}t}$$ } GOING BACK IN TIME

HENCE

$$U_{Ex}(-t)\, U_{Ex}(t) = \mathbb{1}$$

FOR OUR PRESENT FACTORIZATION IN EQ. (1) WE HAVE

$$\tilde{U}(\Delta t) = e^{i\mathcal{L}_q \Delta t} e^{i\mathcal{L}_p \Delta t}$$

$$\tilde{U}(-\Delta t) = e^{-i\mathcal{L}_q \Delta t} e^{-i\mathcal{L}_p \Delta t}$$

HENCE

$$\tilde{U}(-\Delta t)\,\tilde{U}(\Delta t) = e^{-i\mathcal{L}_q \Delta t} e^{-i\mathcal{L}_p \Delta t} .$$

$$e^{i\mathcal{L}_q \Delta t} e^{i\mathcal{L}_p \Delta t} \neq \underline{\Pi}$$

IT IS NOT TIME REVERSIBLE

SINCE $\mathcal{L}_q$ AND $\mathcal{L}_p$ DO NOT COMMUTE

THE FACTORIZATION IN EQ. (1) IS CALLED SEMI-IMPLICT EULER ALGORITHM

AN EQUIVALENT VARIANT IS

$$U_{Ex}(\Delta t) = e^{i\mathcal{L}\Delta t} \approx e^{i\mathcal{L}_p \Delta t} e^{i\mathcal{L}_q \Delta t}$$

WHERE WE EXCHANGED $e^{i\mathcal{L}_q \Delta t}$ AND $e^{i\mathcal{L}_p \Delta t}$

NOW LET'S WORKOUT EXPLICITLY THESE TWO ALGORITHMS

LET'S CONSIDER THE ACTION OF $e^{i\mathcal{L}_q \Delta t}$ AND $e^{i\mathcal{L}_p \Delta t}$ ON

AN INITIAL STATE, RECALL THAT

$$i\mathcal{L}\,\phi(q,p)\Big|_{\substack{q=q(t)\\p=p(t)}} = \dot{\phi}(q(t),p(t))$$

$$\Downarrow$$

$$e^{i\mathcal{L}t}\,\phi(q(0),p(0)) = \phi(q(t),p(t))$$

$e^{i\mathcal{L}t}$ ↑ THE EVOLUTION OPERATOR

$e^{i\mathcal{L}t}$ EVOLVES ϕ OVER A TIME t FROM INITIAL CONDITION $\phi(q(0),p(0))$

I.E. IF $\Gamma(0) = \begin{pmatrix} q(0) \\ p(0) \end{pmatrix}$

$$e^{i\mathcal{L}t}\,\Gamma(0) = \Gamma(t) = \begin{pmatrix} q(t) \\ p(t) \end{pmatrix}$$

NOW IF CONSIDER

$$i\mathcal{L}_q = \sum_i \frac{\vec{p}_i}{m}\frac{\partial}{\partial \vec{q}_i} \quad \text{AND} \quad i\mathcal{L} = \sum_i \vec{F}_i \cdot \frac{\partial}{\partial \vec{p}_i}$$

$$e^{i\mathcal{L}_q \Delta t}\begin{pmatrix} q(0) \\ p(0) \end{pmatrix} = e^{\Delta t \frac{p}{m}\frac{\partial}{\partial q}}\begin{pmatrix} q(0) \\ p(0) \end{pmatrix} =$$

↑ THIS THE LIOUVILLIAN ASSOCIATED TO THE HAMILTONIAN $\mathcal{H}_q = \frac{p^2}{2m}$ (FREE PARTICLE)

SINCE $i\mathcal{L}_q \begin{pmatrix} q \\ p \end{pmatrix} = \begin{pmatrix} \dot{q} \\ \dot{p} \end{pmatrix} = \begin{pmatrix} p/m \\ 0 \end{pmatrix} \Rightarrow \begin{cases} \dot{q} = p/m \\ \dot{p} = 0 \end{cases}$

HENCE WE KNOW EXACTLY THE EVOLUTION OPERATOR, I.E.

$$= \begin{pmatrix} q(0) + \frac{p(0)}{m}\Delta t \\ p(0) \end{pmatrix} = \begin{pmatrix} q(\Delta t) \\ p(0) \end{pmatrix}$$

AND SIMILARLY

$$e^{i\mathcal{L}_p \Delta t} \begin{pmatrix} q(0) \\ p(0) \end{pmatrix} = e^{\Delta t f \frac{\partial}{\partial p}} \begin{pmatrix} q(0) \\ p(0) \end{pmatrix} =$$

THIS IS THE LIOUVILLIAN ASSOCIATED TO THE HAMILTONIAN $\mathcal{H}_p = V(q)$

SINCE

$$i\mathcal{L}_p \begin{pmatrix} q \\ p \end{pmatrix} = \begin{pmatrix} \dot{q} \\ \dot{p} \end{pmatrix} = \begin{pmatrix} 0 \\ f \end{pmatrix} \Rightarrow \begin{cases} \dot{q} = 0 \\ \dot{p} = -\frac{\partial V}{\partial q} \end{cases}$$

$$= \begin{pmatrix} q(0) \\ p(0) + \Delta t f(q(0)) \end{pmatrix} = \begin{pmatrix} q(0) \\ p(\Delta t) \end{pmatrix}$$

ALTERNATIVELY WE CAN FORMALLY REGARD $e^{i\mathcal{L}_q \Delta t}$ AND $e^{i\mathcal{L}_p \Delta t}$ AS OPERATORS ACTING ON FUNCTIONS OF (q,p), I.E.

$$e^{a(p)\frac{\partial}{\partial q}} f(q) = \sum_{n=0}^{\infty} \frac{a^n}{n!} \frac{\partial^n f}{\partial q^n}(q) =$$

TAYLOR EXPANDING THIS EXPONENTIAL

$$= f(q + a(p))$$

SINCE IT IS A TAYLOR EXPANSION AROUND q

AND SIMILARLY

$$\boxed{e^{b(q)\frac{\partial}{\partial p}}\, g(p)} = \sum_{n=0}^{\infty} \frac{b^n}{n!} \frac{\partial^n}{\partial q^n}\, g(p) =$$

$$= \boxed{g(p + b(q))}$$

NOW CONSIDER THE ACTION ON $\begin{pmatrix} q \\ p \end{pmatrix}$:

$$e^{i\mathcal{L}_q \Delta t} = e^{\Delta t \frac{p}{m} \frac{\partial}{\partial q}} = e^{a(p)\frac{\partial}{\partial q}}$$

WITH $a(p) = \frac{\Delta t\, p}{m}$

HENCE

$$\boxed{e^{i\mathcal{L}_q \Delta t} \begin{pmatrix} q \\ p \end{pmatrix} = e^{\Delta t \frac{p}{m} \frac{\partial}{\partial q}} \begin{pmatrix} q \\ p \end{pmatrix} = \begin{pmatrix} q + \Delta t \frac{p}{m} \\ p \end{pmatrix}}$$

AND

$$e^{i\mathcal{L}_p \Delta t} = e^{f(q)\Delta t \frac{\partial}{\partial p}} = e^{b(q)\frac{\partial}{\partial p}}$$

WITH $b(q) = f(q)\,\Delta t$

HENCE

$$\boxed{e^{i\mathcal{L}_p \Delta t} \begin{pmatrix} q \\ p \end{pmatrix} = e^{f(q)\Delta t \frac{\partial}{\partial p}} \begin{pmatrix} q \\ p \end{pmatrix} = \begin{pmatrix} q \\ p + f(q)\Delta t \end{pmatrix}}$$

SEMI-IMPLICIT EULER ALGORITHM

$$e^{i\mathcal{L}_q \Delta t}\, e^{i\mathcal{L}_p \Delta t} \begin{pmatrix} q(0) \\ p(0) \end{pmatrix} =$$

TREAT THESE TWO OPERATOR AS TIME EVOLUTION OPERATORS, SO THAT:

$$e^{i\mathcal{L}_q \Delta t} \begin{pmatrix} q(0) \\ \underbrace{p(0) + F(0)\Delta t}_{p(\Delta t)} \end{pmatrix} =$$

$$= \begin{pmatrix} q(0) + \dfrac{p(\Delta t)}{m}\Delta t \\ p(0) + f(0)\Delta t \end{pmatrix}$$

I.E.

$$\begin{cases} \vec{v}_i(t+\Delta t) = \vec{v}_i(t) + \vec{a}_i(t)\Delta t \\ \vec{r}_i(t+\Delta t) = \vec{r}_i(t) + \vec{v}_i(t+\Delta t)\Delta t \end{cases}$$

NOTE THAT IF WE TREAT FORMALLY $e^{i\mathcal{L}_q \Delta t}$ AND $e^{i\mathcal{L}_p \Delta t}$ AS OPERATORS ACTING ON FUNCTIONS OF q AND p, WE NEED TO APPLY OPERATORS IN INVERSE ORDER TO RECOVER THE SAME ALGORITHM, SINCE WE OPERATE RECURSIVELY RATHER THAN ITERATIVELY

I. E.

$$e^{i\mathcal{L}_p \Delta t}\, e^{i\mathcal{L}_q \Delta t} \begin{pmatrix} q \\ p \end{pmatrix} = \begin{pmatrix} e^{i\mathcal{L}_p \Delta t}\, e^{i\mathcal{L}_q \Delta t}\, q \\ e^{i\mathcal{L}_p \Delta t}\, e^{i\mathcal{L}_q \Delta t}\, p \end{pmatrix} =$$

FUNCTIONS OF (q,p)

FUNCTION OF (q,p)

$$= \begin{pmatrix} e^{i\mathcal{L}_p \Delta t} \left(q + \frac{p}{m} \Delta t\right) \\ e^{i\mathcal{L}_p \Delta t}\, p \end{pmatrix} = \begin{pmatrix} q + \frac{p + F(q)\Delta t}{m} \Delta t \\ p + F(q)\Delta t \end{pmatrix} =$$

$p(\Delta t) = v(\Delta t)\, m$

$$= \begin{pmatrix} p + F(q)\Delta t \\ q + v(\Delta t)\Delta t \end{pmatrix}$$

AND NOW ITS VARIANT

$$e^{i\mathcal{L}_p \Delta t}\, e^{i\mathcal{L}_q \Delta t} \begin{pmatrix} q(0) \\ p(0) \end{pmatrix} =$$

$q(\Delta t)$

$$= e^{i\mathcal{L}_p \Delta t} \begin{pmatrix} q(0) + \frac{p(0)}{m} \Delta t \\ p(0) \end{pmatrix} =$$

$$= \begin{pmatrix} q(0) + \frac{p(0)}{m} \Delta t \\ p(0) + f(q(\Delta t))\, \Delta t \end{pmatrix}$$

$$\begin{cases} \vec{r}_i(t+\Delta t) = \vec{r}_i(t) + \vec{v}_i(t)\,\Delta t \\ \vec{v}_i(t+\Delta t) = \vec{v}_i(t) + \vec{a}_i(\vec{r}_1(t+\Delta t)\ldots\vec{r}_N(t+\Delta t))\Delta t \end{cases}$$

TREATING $e^{i\mathcal{L}_q \Delta t}$ AND $e^{i\mathcal{L}_p \Delta t}$ FORMALLY AS OPERATOR:

WE NEED TO INVERT ORDER OF OPERATORS ✓ FUNCTIONS OF (q,p)

$$e^{i\mathcal{L}_q \Delta t}\, e^{i\mathcal{L}_p \Delta t} \begin{pmatrix} q \\ p \end{pmatrix} = \begin{pmatrix} e^{i\mathcal{L}_q \Delta t} e^{i\mathcal{L}_p \Delta t}\, q \\ e^{i\mathcal{L}_q \Delta t} e^{i\mathcal{L}_p \Delta t}\, p \end{pmatrix} =$$

$$= \begin{pmatrix} e^{i\mathcal{L}_q \Delta t}\, q \\ e^{i\mathcal{L}_q \Delta t}[p + f(q)\Delta t] \end{pmatrix} = \begin{pmatrix} q + \frac{p}{m}\Delta t \\ p + f\left(q + \frac{p}{m}\Delta t\right) \end{pmatrix}$$

WHICH IS THE SAME ALGORITHM ABOVE

SYMPLECTICITY OF SEMI-IMPLICIT EULER ALGORITHMS

THESE TWO ALGORITHMS ARE

$$e^{i\mathcal{L}_q \Delta t}\, e^{i\mathcal{L}_p \Delta t}\, \Gamma(0) \qquad (E1)$$

$$e^{i\mathcal{L}_p \Delta t}\, e^{i\mathcal{L}_q \Delta t}\, \Gamma(0) \qquad (E2)$$

WHERE $\Gamma(0) = \begin{pmatrix} q(0) \\ p(0) \end{pmatrix}$

AN APPROXIMATE TIME EVOLUTION OPERATOR $\tilde{U}(\Delta t)$, I.E A FINITE-DIFFERENCE ALGORITHM, IS SAID TO BE SYMPLECTIC IF THE MAPPING THAT IT INDUCES $\phi_{FD}(t, X_0)$ IS SYMPLECTIC.

ALGORITHMS (E1) AND (E2) ARE SYMPLECTIC ?

YES, SINCE $e^{i\mathcal{L}_q \Delta t}$ AND $e^{i\mathcal{L}_p \Delta t}$ ARE TIME EVOLUTION OPERATORS ASSOCIATED TO THE HAMILTONIANS $\mathcal{H}_q = \frac{p^2}{2m}$ AND $\mathcal{H}_p = V(q)$ RESPECTIVELY, HENCE THEY BOTH INDUCE A SYMPLECTIC MAPPING THUS HAVING OVERALL A SYMPLECTIC MAPPING.

E.G. CONSIDER (E1)

$$\phi_{E1}(\Delta t, x_0) = \phi_q(\Delta t, \phi_p(\Delta t, x_0))$$

- ϕ_{E1}: MAPPING INDUCED BY (E1)
- ϕ_q: MAPPING INDUCED BY $e^{i\mathcal{L}_q \Delta t}$
- ϕ_p: MAPPING INDUCED BY $e^{i\mathcal{L}_p \Delta t}$

WHERE

$\phi_p(\Delta t, x_0)$ IS THE MAPPING INDUCED BY $e^{i\mathcal{L}_p \Delta t}$ AND

$\phi_q(\Delta t, x_0)$ IS THAT INDUCED BY $e^{i\mathcal{L}_q \Delta t}$

HENCE

$$M_{E1} = \frac{\partial \phi_{E1}}{\partial x_0} = \frac{\partial \phi_q}{\partial x_0}\Big|_{x=\phi_p(\Delta t, x_0)} \frac{\partial \phi_p}{\partial x_0} = M_q M_p$$

THE SYMPLECTIC CONDITION FOR (E1) READS:

$$M_{E1} J {}^t M_{E1} = J$$

I.E.

$$M_q M_p J {}^t M_p {}^t M_q = J$$

BUT $e^{i f_p \Delta t}$ IS SYMPLECTIC, THEREFORE

$$M_p J {}^t M_p = J \quad \Rightarrow \quad M_q J {}^t M_q = J$$

WHICH IS SATISFIED SINCE ALSO $e^{i f_q \Delta t}$ IS SYMPLECTIC

ENERGY FLUCTUATIONS

FOR SEMI-IMPLICT EULER ALGORITHMS WE HAVE SHOWN THAT

$$\tilde{U}(\Delta t) = U_{ex}(\Delta t) + O(\Delta t^2)$$

LET'S CONSIDER THE GENERAL CASE WHERE

$$\tilde{U}(\Delta t) = U_{ex}(\Delta t) + O(\Delta t^k)$$

BE $E(t)$ THE CONSERVED ENERGY AT TIME t, I.E.

$$E(t) = \sum_{i=1}^{N} \frac{\vec{p}_i^{\,2}(t)}{2m} + V(\vec{q}_1(t) \dots \vec{q}_N(t))$$

THEN:

$$U_{ex}(t)\ E(0) = E(t) = E(0)$$

HENCE IF $t = n\Delta t$

$$\tilde{U}(t)\ E(0) = \left[\tilde{U}(\Delta t)\right]^n E(0) =$$

$$= \left[U_{ex}(\Delta t) + O(\Delta t^k)\right]^n E(0) =$$

$$= \left[U_{ex}(\Delta t)\right]^n \left[\mathbb{1} + U_{ex}^{-1}(\Delta t)\, O(\Delta t^k)\right]^n E(0) =$$

$$\approx \left[U_{ex}(\Delta t)\right]^n \left[\mathbb{1} + n\, U_{ex}(-\Delta t)\, O(\Delta t^k)\right] E(0) =$$

BUT $\left[U_{ex}(\Delta t)\right]^n = U_{ex}(t)$ THEN

$$= \left[U_{ex}(t) + n\, U_{ex}(t)\, U_{ex}(-\Delta t)\, O(\Delta t^k)\right] E(0) =$$

$$U_{ex}(t)\, U_{ex}(-\Delta t) = U_{ex}(t - \Delta t)$$

SO THAT WE HAVE

$$\tilde{U}(t)\ E(0) = E(0) + n\, U_{ex}(t - \Delta t)\, O(\Delta t^k) E(0)$$

$$= E(0) + \underbrace{t\, U_{ex}(t - \Delta t)\, O(\Delta t^{k-1})}\, E(0)$$

NOTE THAT THIS IS AN OPERATOR AND WE DO NOT KNOW ITS FULL TIME DEPENDENCE BUT IF t IS FIXED IT SCALES AS $\alpha \Delta t^k$

$$\tilde{E}(t) - E(0) = t\, O(\Delta t^{k-1})$$

FOR SEMI-IMPLICIT EULER ALGORITHMS WE HAVE $K = 2$ HENCE ENERGY FLUCTUATIONS ARE $\propto \mathcal{O}(\Delta t)$.

$$\sigma(E) \equiv \langle [\tilde{E}(t) - E(0)]^2 \rangle^{1/2} =$$

$\langle \ldots \rangle$ TIME AVERAGE

$$= \left(\frac{1}{T} \int_0^T [\tilde{E}(t) - E(0)]^2 dt \right)^{1/2} =$$

$$= \left(\frac{1}{T} \int_0^T [t\, \mathcal{O}(\Delta t^{K-1})]^2 dt \right)^{1/2} =$$

$$= \frac{T}{\sqrt{3}} \mathcal{O}(\Delta t^{K-1}) \propto T\, \mathcal{O}(\Delta t^{K-1}) \quad (F1)$$

HENCE FOR SEMI-IMPLICIT EULER ALGORITHMS:

$\sigma(E) \propto \mathcal{O}(\Delta t)$ I.E. IT'S LINEAR IN Δt

HOW TO TEST AN ALGORITHM IMPLEMENTATION

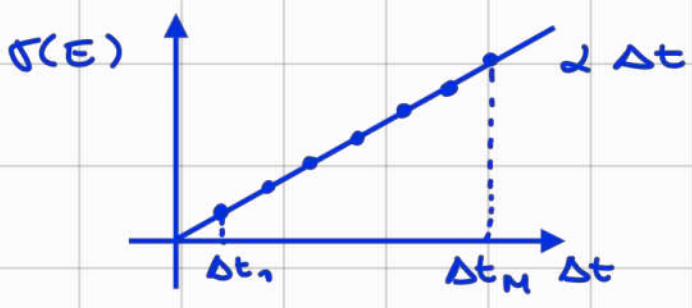
PERFORM A SERIES OF M SIMULATIONS WHERE Δt_ℓ AND n_ℓ ARE THE TIME STEP AND NUMBER OF STEPS OF ℓ-th SIMULATION, RESPECTIVELY, WITH $n_\ell = \frac{T}{\Delta t_\ell}$ SO THAT THE TOTAL SIMULATION TIME IS FIXED, AND

$\Delta t_1 < \Delta t_2 \dots < \Delta t_M$

IN THIS WAY ACCORDING TO EQ. (F1) $\sigma(E) \propto \Delta t^{k-1}$

SIMULATION	TIME-STEP	SIMULATION STEPS
# 1	$\Delta t = \Delta t_1$	$n_1 = \frac{T}{\Delta t_1}$
⋮		
# M	$\Delta t = \Delta t_M$	$n_M = \frac{T}{\Delta t_M}$

IF WE HAVE A SEMI-EULER ALGORITHM $\sigma(E) \propto \Delta t$ THEN WE EXPECT



ENERGY DRIFT: SHADOW HAMILTONIAN

FOR A SYMPLECTIC ALGORITH THERE ALWAYS EXISTS A SHADOW HAMILTONIAN $\mathcal{H}_S$ SUCH THAT

$$e^{i\mathcal{L}_S \Delta t} = \tilde{U}(\Delta t)$$

E.G. $\tilde{U} = e^{i\mathcal{L}_q \Delta t} e^{i\mathcal{L}_p \Delta t}$ SEMI-EULER

WHERE

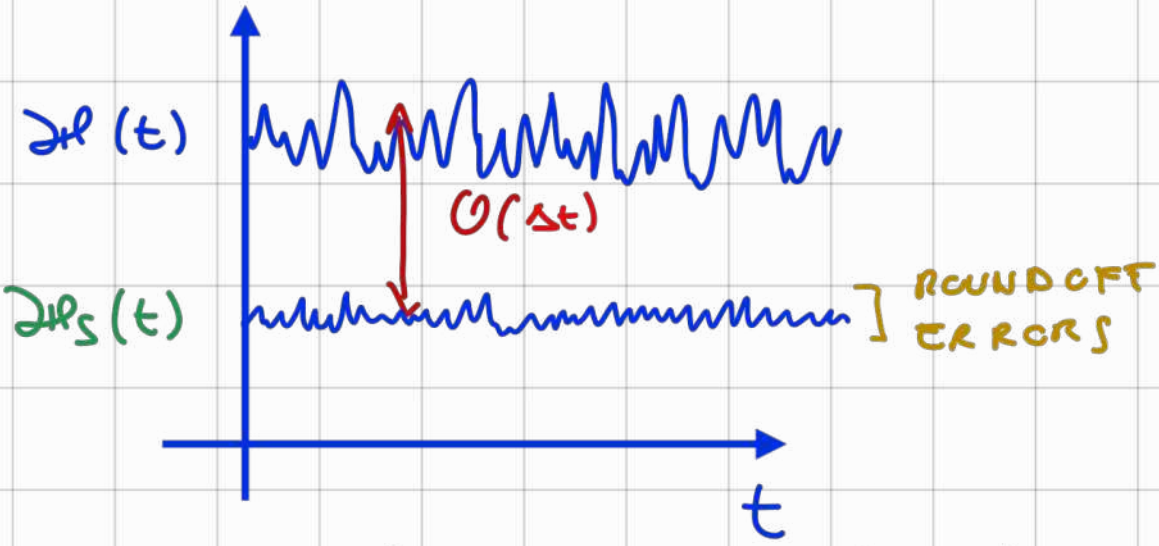
$$i\mathcal{L}_S = \frac{\partial \mathcal{H}_S}{\partial p}\frac{\partial}{\partial q} - \frac{\partial \mathcal{H}_S}{\partial q}\frac{\partial}{\partial p}$$

I.E. IT IS THE LIOUVILLIAN ASSOCIATED TO $\mathcal{H}_S$.

HENCE $\tilde{U}(\Delta t)\,\mathcal{H}_S = \mathcal{H}_S$ I.E

IT IS EXACTLY CONSERVED

THIS IS WHY SYMPLECTIC ALGORITHS DO NOT EXHIBIT ENERGY DRIFT



$$\mathcal{H}_S(t) - \mathcal{H}(t) = O(\Delta t)$$

NOTE THAT THIS IMPLIES THAT ENERGY FLUCTUATIONS SCALES AS Δt

CASE OF SEMI-IMPLICIT EULER

CONSIDER THE HAMILTONIAN

$$\mathcal{H} = \frac{p^2}{2m} + V(q)$$

SO THAT

$$i\mathcal{L}_q = \frac{\partial \mathcal{H}}{\partial p}\frac{\partial}{\partial q} = \frac{p}{m}\frac{\partial}{\partial q} \quad \text{AND}$$

$$i\mathcal{L}_p = -\frac{\partial \mathcal{H}}{\partial q}\frac{\partial}{\partial p} = f(q)\frac{\partial}{\partial p}$$

CONSIDER THE BCH FORMULA

$$e^{\hat{x}}e^{\hat{y}} = e^{\hat{x}+\hat{y}+\frac{1}{2}[\hat{x},\hat{y}]+\frac{1}{12}([\hat{x},[\hat{x},\hat{y}]]+[\hat{y},[\hat{y},\hat{x}]])+\cdots}$$

WITH $\hat{x} = i\mathcal{L}_q \Delta t \quad \hat{y} = i\mathcal{L}_p \Delta t$

WE HAVE

$$\underbrace{e^{i\mathcal{L}_q \Delta t}\, e^{i\mathcal{L}_p \Delta t}}_{\text{SEMI-IMPLICIT EULER (E2) SINCE } e^{i\mathcal{L}_q} \text{ AND } e^{i\mathcal{L}_p} \text{ ARE OPERATORS HERE}} = e^{i(\mathcal{L}_p+\mathcal{L}_q)\Delta t + \frac{\Delta t^2}{2}[i\mathcal{L}_q, i\mathcal{L}_p]+\cdots} =$$

$$= e^{i\mathcal{L}_S \Delta t} =$$

NOTE THAT $\frac{\partial}{\partial q}\frac{\partial}{\partial p}$ TERMS CANCEL

$$= e^{i(\mathcal{L}_p+\mathcal{L}_q)\Delta t + \frac{\Delta t^2}{2}\left[\frac{\partial \mathcal{H}}{\partial p}\frac{\partial}{\partial q}, -\frac{\partial \mathcal{H}}{\partial q}\frac{\partial}{\partial p}\right] + \mathcal{O}(\Delta t^3)} =$$

$$= e^{i\mathcal{L}\Delta t + \frac{\Delta t^2}{2}\left[-\frac{\partial \mathcal{H}}{\partial p}\frac{\partial^2 \mathcal{H}}{\partial q^2}\frac{\partial}{\partial p} + \frac{\partial \mathcal{H}}{\partial q}\frac{\partial^2 \mathcal{H}}{\partial p^2}\frac{\partial}{\partial q}\right] + \mathcal{O}(\Delta t^3)}$$

WHERE $\mathcal{L}_S$ IS THE LIOUVILLIAN OPERATOR ASSOCIATED TO THE SHADOW HAMILTONIAN

HENCE UP TO $\mathcal{O}(\Delta t^2)$ THE SHADOW HAMILTONIAN IS

$$\mathcal{H}_S = \mathcal{H} + \frac{\Delta t}{2}\frac{\partial \mathcal{H}}{\partial p}\frac{\partial \mathcal{H}}{\partial q} + \mathcal{O}(\Delta t^2)$$

INDEED

$$i\mathcal{L}_S = i\mathcal{L}_q + i\mathcal{L}_p + \frac{\Delta t}{2}\left[\frac{\partial^2 \mathcal{H}}{\partial p^2}\frac{\partial \mathcal{H}}{\partial q}\frac{\partial}{\partial q} + \right.$$

$$- \frac{\partial^2 \mathcal{H}}{\partial q^2}\frac{\partial \mathcal{H}}{\partial p}\frac{\partial}{\partial p} + \frac{\partial \mathcal{H}}{\partial p}\frac{\partial \mathcal{H}}{\partial q}\frac{\partial}{\partial q} +$$

$$\left. - \frac{\partial \mathcal{H}}{\partial q}\frac{\partial \mathcal{H}}{\partial p}\frac{\partial}{\partial p}\right] + \mathcal{O}(\Delta t^2) =$$

$$= i\mathcal{L}_q + i\mathcal{L}_p + \frac{\Delta t}{2}\left[-\frac{\partial^2 \mathcal{H}}{\partial q^2}\frac{\partial \mathcal{H}}{\partial p}\frac{\partial}{\partial p} + \frac{\partial^2 \mathcal{H}}{\partial p^2}\frac{\partial \mathcal{H}}{\partial q}\frac{\partial}{\partial q}\right] +$$

$$\mathcal{O}(\Delta t^2)$$

NOTE THAT:

$$\mathcal{H}_S = \mathcal{H}\boxed{- \frac{\Delta t}{2}\sum_i^N \frac{\vec{p}_i}{m_i}\cdot\vec{f}_i} + \mathcal{O}(\Delta t^2) \qquad (HS2)$$

IF WE CONSIDER ALGORITHM (E1)

$$e^{i\mathcal{L}_p \Delta t}\, e^{i\mathcal{L}_q \Delta t}$$

$$= e^{i(\mathcal{L}_p + \mathcal{L}_q)\Delta t} + \frac{\Delta t^2}{2}\boxed{\left[-\frac{\partial \mathcal{H}}{\partial q}\frac{\partial}{\partial p}, \frac{\partial \mathcal{H}}{\partial p}\frac{\partial}{\partial q}\right]} + \mathcal{O}(\Delta t^3) \qquad (LS1)$$

$$= e^{i\mathcal{L}_S \Delta t} \qquad \| \; -\frac{\Delta t^2}{2}\left[\frac{\partial \mathcal{H}}{\partial p}\frac{\partial}{\partial q}, -\frac{\partial \mathcal{H}}{\partial q}\frac{\partial}{\partial p}\right]$$

HENCE WE HAVE JUST TO CHANGE SIGN IN $\mathcal{O}(\Delta t)$ TERM IN EQ. (HS2) I.E.

$$\mathcal{H}_S = \mathcal{H}\boxed{+ \frac{\Delta t}{2}\sum_i^N \frac{\vec{p}_i}{m_i}\cdot\vec{f}_i} + \mathcal{O}(\Delta t^2) \qquad (HS1)$$

→ atomsim/

SEE README

EXAMPLE CONSIDER THE HARMONIC OSCILLATOR

$$\mathcal{H}(q,p) = \frac{p^2}{2m} + \frac{k}{2} q^2$$

AND EULER SEMI IMPLICIT ALGORITHM (E1)
FROM EQS. (LS1) AND (MS1)

$$i\mathcal{L}_S = \frac{p}{m}\frac{\partial}{\partial q} - kq\frac{\partial}{\partial p} + \frac{k\Delta t}{2m} q \frac{\partial}{\partial q} - \frac{k\Delta t}{2m} p \frac{\partial}{\partial p}$$

$$\mathcal{H}_S(q,p) = \frac{p^2}{2m} + \frac{k}{2} q^2 - \frac{k\Delta t}{2m} qp$$

ANYWAY WE CAN PROVE THAT
THIS HAMILTONIAN IS EXACTLY
CONSERVED BY THE SEMI-IMPLICIT
EULER ALGORITHM (E1)
INDEED

$$e^{i\mathcal{L}_p \Delta t} e^{i\mathcal{L}_q \Delta t} \mathcal{H}_S(q,p) =$$

$$e^{i\mathcal{L}_p \Delta t} e^{i\mathcal{L}_q \Delta t} \left(\frac{p^2}{2m} + \frac{1}{2} k q^2 - \frac{\Delta t}{2}\frac{k}{m} qp \right) =$$

REMEMBERING THAT:

$$e^{i\mathcal{L}_q \Delta t} = e^{\frac{p}{m}\Delta t \frac{\partial}{\partial q}}$$

$$e^{i\mathcal{L}_p \Delta t} = e^{-kq\Delta t \frac{\partial}{\partial p}}$$

WE HAVE ← THIS IS ALGORITH (E1)

$$e^{i\mathcal{L}_p \Delta t} e^{i\mathcal{L}_q \Delta t} \mathcal{H}_S(q,p) =$$

$$e^{i\mathcal{L}_P \Delta t}\left[\frac{p^2}{2m} + \frac{1}{2}k\left(q + \frac{p}{m}\Delta t\right)^2 - \alpha\left(q + \frac{p}{m}\Delta t\right)p\right]$$

WHERE $\alpha \equiv \frac{\Delta t\, k}{2m}$

$$= \frac{1}{2m}\left(\left(p - kq\Delta t\right)^2 + \frac{1}{2}k\left(q + (p - kq\Delta t)\frac{\Delta t}{m}\right)^2 + \right.$$

$$\left. - \alpha\left(q + (p - kq\Delta t)\frac{\Delta t}{m}\right)\left(p - kq\Delta t\right)\right) =$$

$$= \frac{p^2}{2m} + \frac{k}{2}q^2 - \frac{k\Delta t}{2m}qp = \mathcal{H}_S(q,p)$$

I.E. $\mathcal{H}_S$ IS EXACTLY CONSERVED!