



$$T = \frac{1}{2} m v^2 = \frac{1}{2} m (\dot{x}^2 + \dot{y}^2)$$

$$= \frac{1}{2} m (\dot{r}^2 + r^2 \dot{\theta}^2)$$

$$V = mgy = mg(-r \cos \theta)$$

$$L = T - V = \frac{1}{2} m (\dot{r}^2 + r^2 \dot{\theta}^2) + mgr \cos \theta$$

$$= \frac{1}{2} m l^2 \dot{\theta}^2 + mgl \cos \theta$$

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{\theta}} \right) - \frac{\partial L}{\partial \theta} = 0$$

$$\frac{d}{dt} (m l^2 \dot{\theta}) - mgl(-\sin \theta) = 0$$

$$m l^2 \ddot{\theta} + mgl \sin \theta = 0$$

$$\ddot{\theta} = -\frac{g}{l} \sin \theta$$

← Equation of Motion

Hamiltonian Mechanics

$$H = \text{Total Energy} = T + V \quad (\text{in simple cases})$$

$$= \sum p_i \dot{q}_i - L \quad (\text{in general case})$$

$$p_i = \frac{\partial L}{\partial \dot{q}_i}$$

$$H \text{ in Cartesian Coordinates in simple cases} = T + V = \frac{1}{2m} (p_x^2 + p_y^2 + p_z^2) + V$$

Hamilton's Equations

$$\boxed{\frac{dq_i}{dt} = \frac{\partial H}{\partial p_i} \quad \frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i}}$$

Spring Hamiltonian

$$T = \frac{1}{2m} p_x^2$$

$$V = \frac{1}{2} k x^2$$

$$H = T + V = \frac{1}{2m} p_x^2 + \frac{1}{2} k x^2$$

$$\boxed{\frac{dx}{dt} = \frac{\partial H}{\partial p} = \frac{p_x}{m} \quad \frac{dp_x}{dt} = -\frac{\partial H}{\partial x} = -kx}$$

Just definition of momentum $p = mv$ Hooke's Law $F = -kx$

Pendulum Hamiltonian

$$L = T - V = \frac{1}{2} m (\dot{r}^2 + r^2 \dot{\theta}^2) + mgr \cos \theta$$
$$= \frac{1}{2} m l^2 \dot{\theta}^2 + mgl \cos \theta$$

$$H = p_{\theta} \dot{\theta} - L = \left(\frac{p_{\theta}^2}{m l^2} \right) - \left(\frac{1}{2} m l^2 \dot{\theta}^2 + mgl \cos \theta \right)$$
$$= \left(\frac{p_{\theta}^2}{m l^2} \right) - \left(\frac{p_{\theta}^2}{2 m l^2} + mgl \cos \theta \right)$$

$$\boxed{H = \frac{1}{2 m l^2} p_{\theta}^2 - mgl \cos \theta}$$

Same Eqn. we got from Lagrangian mechanics

$$p_{\theta} = \frac{\partial L}{\partial \dot{\theta}} = m l^2 \dot{\theta} \Rightarrow \dot{\theta} = \frac{p_{\theta}}{m l^2}$$

$$\frac{d\theta}{dt} = \frac{\partial H}{\partial p_{\theta}} = \frac{p_{\theta}}{m l^2}$$

$$\frac{dp_{\theta}}{dt} = - \frac{\partial H}{\partial \theta} = -mgl \sin \theta$$

$$\downarrow$$
$$\frac{dp_{\theta}}{dt} = \frac{d}{dt} \left(m l^2 \frac{d\theta}{dt} \right) = m l^2 \ddot{\theta}$$

$$m l^2 \ddot{\theta} = -mgl \sin \theta$$

$$\boxed{\ddot{\theta} = -\frac{g}{l} \sin \theta}$$

Canonical Transformation

$$\frac{dq_i}{dt} = \frac{\partial H}{\partial p_i} \quad \frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i} \implies \frac{dQ_i}{dt} = \frac{\partial H}{\partial P_i} \quad \frac{dP_i}{dt} = -\frac{\partial H}{\partial Q_i}$$

$Q_i(q_i, p_i)$ and $P_i(q_i, p_i)$ are our new coordinates. They are functions of the old coordinates. We can go the other way with $q_i(Q_i, P_i)$ and $p_i(Q_i, P_i)$

Multivariable Chain Rule

$$\frac{d}{dt} f(a, b, c, \dots) = \frac{\partial f}{\partial a} \frac{da}{dt} + \frac{\partial f}{\partial b} \frac{db}{dt} + \frac{\partial f}{\partial c} \frac{dc}{dt} + \dots$$

$$\begin{aligned} \frac{dQ_i}{dt} &= \sum \frac{\partial Q_i}{\partial q_j} \frac{dq_j}{dt} + \frac{\partial Q_i}{\partial p_j} \frac{dp_j}{dt} \\ &\quad + \cancel{\frac{\partial Q_i}{\partial t} \frac{dt}{dt}} \\ \frac{dP_i}{dt} &= \sum \frac{\partial P_i}{\partial q_j} \frac{dq_j}{dt} + \frac{\partial P_i}{\partial p_j} \frac{dp_j}{dt} \\ &\quad + \cancel{\frac{\partial P_i}{\partial t} \frac{dt}{dt}} \end{aligned}$$

For a 1-D system, we have

If we wanted Q_i and P_i to also be an explicit function of time, we would need these terms.

$$\begin{bmatrix} \dot{Q} \\ \dot{P} \end{bmatrix} = \begin{bmatrix} \frac{\partial Q}{\partial q} & \frac{\partial Q}{\partial p} \\ \frac{\partial P}{\partial q} & \frac{\partial P}{\partial p} \end{bmatrix} \begin{bmatrix} \dot{q} \\ \dot{p} \end{bmatrix}$$

By Hamilton's Equations, we have

$$\begin{bmatrix} \dot{q} \\ \dot{p} \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \begin{bmatrix} \frac{\partial H}{\partial q} \\ \frac{\partial H}{\partial p} \end{bmatrix}$$

$$\begin{bmatrix} \dot{Q} \\ \dot{P} \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \begin{bmatrix} \frac{\partial H}{\partial Q} \\ \frac{\partial H}{\partial P} \end{bmatrix}$$

$$\begin{bmatrix} \dot{q} \\ \dot{p} \end{bmatrix} = \begin{bmatrix} \frac{\partial Q}{\partial q} & \frac{\partial Q}{\partial p} \\ \frac{\partial P}{\partial q} & \frac{\partial P}{\partial p} \end{bmatrix} \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \begin{bmatrix} \frac{\partial H}{\partial q} \\ \frac{\partial H}{\partial p} \end{bmatrix}$$

Last Step

$$\begin{aligned} \frac{\partial H}{\partial q} &= \frac{\partial H}{\partial Q} \frac{\partial Q}{\partial q} + \frac{\partial H}{\partial P} \frac{\partial P}{\partial q} \\ \frac{\partial H}{\partial p} &= \frac{\partial H}{\partial Q} \frac{\partial Q}{\partial p} + \frac{\partial H}{\partial P} \frac{\partial P}{\partial p} \end{aligned} \implies \begin{bmatrix} \frac{\partial H}{\partial q} \\ \frac{\partial H}{\partial p} \end{bmatrix} = \begin{bmatrix} \frac{\partial Q}{\partial q} & \frac{\partial P}{\partial q} \\ \frac{\partial Q}{\partial p} & \frac{\partial P}{\partial p} \end{bmatrix} \begin{bmatrix} \frac{\partial H}{\partial Q} \\ \frac{\partial H}{\partial P} \end{bmatrix}$$

$$\begin{bmatrix} \dot{Q} \\ \dot{P} \end{bmatrix} = \begin{bmatrix} \frac{\partial Q}{\partial q} & \frac{\partial Q}{\partial p} \\ \frac{\partial P}{\partial q} & \frac{\partial P}{\partial p} \end{bmatrix} \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \begin{bmatrix} \frac{\partial H}{\partial Q} \\ \frac{\partial H}{\partial P} \end{bmatrix}$$

If you're doing Physics.

If you're doing math.

$$M = \text{Jacobian} = \begin{bmatrix} \frac{\partial Q}{\partial q} & \frac{\partial Q}{\partial p} \\ \frac{\partial P}{\partial q} & \frac{\partial P}{\partial p} \end{bmatrix}$$

$$J = \Omega = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$$

By Hamilton's Equations,

$$\begin{bmatrix} \dot{Q} \\ \dot{P} \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \begin{bmatrix} \frac{\partial H}{\partial Q} \\ \frac{\partial H}{\partial P} \end{bmatrix}$$

$$M J M^T = J \text{ for a canonical transform.}$$

Testing if Euler Methods are Canonical Using Springs

$\frac{dp}{dt} = -kx$ and $\frac{dx}{dt} = \frac{p}{m}$ are the equations of motion

Euler

$$\begin{aligned} x_{n+1} &= x_n + \Delta t \frac{dx}{dt} = x_n + \Delta t \frac{p_n}{m} \\ p_{n+1} &= p_n + \Delta t \frac{dp}{dt} = p_n - \Delta t k x_n \end{aligned} \Rightarrow \text{Jacobian} = \begin{bmatrix} \frac{dx_{n+1}}{dx_n} & \frac{dx_{n+1}}{dp_n} \\ \frac{dp_{n+1}}{dx_n} & \frac{dp_{n+1}}{dp_n} \end{bmatrix} = \begin{bmatrix} 1 & \frac{\Delta t}{m} \\ -\Delta t k & 1 \end{bmatrix} = M$$

$$M J M^T = \begin{bmatrix} 1 & \frac{\Delta t}{m} \\ -\Delta t k & 1 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \begin{bmatrix} 1 & \frac{\Delta t}{m} \\ -\Delta t k & 1 \end{bmatrix} = \left(1 + \frac{k}{m} \Delta t^2\right) \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \neq \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$$

Euler is not canonical.

Semi-Implicit Euler v1

$$\begin{aligned} x_{n+1} &= x_n + \Delta t \frac{dx}{dt} = x_n + \Delta t \frac{p_{n+1}}{m} = x_n + \Delta t \frac{1}{m} (p_n - \Delta t k x_n) = x_n + \Delta t \frac{p_n}{m} - \frac{1}{m} \Delta t^2 k x_n \\ p_{n+1} &= p_n + \Delta t \frac{dp}{dt} = p_n - \Delta t k x_n = \left(1 - \frac{1}{m} \Delta t^2 k\right) p_n + \Delta t \frac{p_n}{m} \end{aligned}$$

$$\text{Jacobian is } \begin{bmatrix} \frac{dx_{n+1}}{dx_n} & \frac{dx_{n+1}}{dp_n} \\ \frac{dp_{n+1}}{dx_n} & \frac{dp_{n+1}}{dp_n} \end{bmatrix} = \begin{bmatrix} 1 - \frac{k}{m} \Delta t^2 & \frac{\Delta t}{m} \\ -k \Delta t & 1 \end{bmatrix} = M$$

$$M J M^T = \left(1 - \frac{k}{m} \Delta t^2 - \left(-\frac{k}{m} \Delta t^2\right)\right) J = J$$

Semi-Implicit Euler v1 is canonical

Semi-Implicit Euler v2

$$\begin{aligned} x_{n+1} &= x_n + \Delta t \frac{dx}{dt} = x_n + \frac{p_n}{m} \Delta t \\ p_{n+1} &= p_n + \Delta t \frac{dp}{dt} = p_n + \Delta t (-k x_{n+1}) = p_n - k \Delta t \left(x_n + \frac{p_n}{m} \Delta t\right) = \left(1 - \frac{k}{m} \Delta t^2\right) p_n - k \Delta t x_n \end{aligned}$$

$$\text{Jacobian} = \begin{bmatrix} 1 & \frac{\Delta t}{m} \\ -k \Delta t & 1 - \frac{k}{m} \Delta t^2 \end{bmatrix} = M$$

$$M J M^T = \left(1 - \frac{k}{m} \Delta t^2 - \left(-\frac{k}{m} \Delta t^2\right)\right) J = J$$

Semi-Implicit Euler v2 is canonical.

Arbitrary Function of Position and Momentum \rightarrow Arbitrary Function of Time

$F(p_i, q_i) \rightarrow F(t)$ For example, $F = \vec{L} = \vec{q} \times \vec{p}$, where \vec{L} is angular momentum.

$$F(p_i, q_i) = \begin{bmatrix} p_i \\ \vdots \\ q_i \\ \vdots \end{bmatrix} \text{ eventually } x$$
$$\frac{dF}{dt} = \sum \frac{\partial F}{\partial q_i} \frac{dq_i}{dt} + \frac{\partial F}{\partial p_i} \frac{dp_i}{dt} + \frac{\partial F}{\partial t} \frac{dt}{dt}$$

If F were also an explicit function of time,

$$\frac{dF}{dt} = \sum \frac{\partial F}{\partial q_i} \frac{\partial H}{\partial p_i} - \frac{\partial F}{\partial p_i} \frac{\partial H}{\partial q_i}$$
$$\frac{dq_i}{dt} = \frac{\partial H}{\partial p_i} \quad \frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i} \rightarrow$$

Poisson Bracket

$$\{F, G\} = \sum \frac{\partial F}{\partial q_i} \frac{\partial G}{\partial p_i} - \frac{\partial F}{\partial p_i} \frac{\partial G}{\partial q_i} \Rightarrow \frac{dF}{dt} = \{F, H\}$$

Rules of Poisson Algebra

1. $\{X, Y\} = -\{Y, X\}$ — Anticommutativity
2. $\{aX + bY, Z\} = a\{X, Z\} + b\{Y, Z\}$
 $\{X, aY + bZ\} = a\{X, Y\} + b\{X, Z\}$ — Bilinearity
3. $\{XY, Z\} = \{X, Z\}Y + X\{Y, Z\}$ — Leibniz Rule
4. $\{X, \{Y, Z\}\} + \{Y, \{Z, X\}\} + \{Z, \{X, Y\}\} = 0$ — Jacobi Identity

If in canonical coordinates

$$\begin{aligned} 5. \{p_i, p_j\} &= 0 \\ \{q_i, q_j\} &= 0 \\ \{q_i, p_j\} &= \begin{cases} 1 & \text{if } i=j \\ 0 & \text{else} \end{cases} \end{aligned}$$

Important Consequences

$$\{F(q_i, p_i), p_i\} = \frac{\partial F}{\partial q_i} = -\{p_i, F(q_i, p_i)\}$$

and

$$\{q_i, F(q_i, p_i)\} = \frac{\partial F}{\partial p_i} = -\{F(q_i, p_i), q_i\}$$

Lie Series

Start with $f(t) \approx \sum_{k=0}^{\infty} \frac{f^{(k)}(t_0)}{k!} (t-t_0)^k = f(t_0) + \Delta t \frac{df}{dt} + \frac{\Delta t^2}{2!} \frac{d^2 f}{dt^2} + \frac{\Delta t^3}{3!} \frac{d^3 f}{dt^3} + \dots$

Replace time derivatives w/ Poisson Brackets

$$f(t) \approx f(t_0) + \Delta t \{f, H\} + \frac{\Delta t^2}{2!} \{\{f, H\}, H\} + \frac{\Delta t^3}{3!} \{\{\{f, H\}, H\}, H\} + \dots$$

First-order Approximation

$$\begin{bmatrix} q_{n+1} \\ p_{n+1} \end{bmatrix} = \begin{bmatrix} q_n \\ p_n \end{bmatrix} + \Delta t \left\{ \begin{bmatrix} q_n \\ p_n \end{bmatrix}, H \right\} = \begin{bmatrix} q_n \\ p_n \end{bmatrix} + \Delta t \begin{bmatrix} \frac{\partial H}{\partial p_n} \\ -\frac{\partial H}{\partial q_n} \end{bmatrix}$$

↑
Bad Euler

Shift Operator

$$f(t) \approx \sum_{k=0}^{\infty} \frac{(t-t_0)^k}{k!} \frac{d^k f}{dt^k} \rightarrow \left(\sum_{k=0}^{\infty} \frac{\Delta t^k}{k!} \frac{d^k}{dt^k} \right) f(t_0) = f(t_0 + \Delta t)$$

Shift operator

$$\hat{S} = \sum_{k=0}^{\infty} \frac{\Delta t^k}{k!} \frac{d^k}{dt^k} = \sum_{k=0}^{\infty} \frac{\Delta t^k}{k!} \left(\frac{d}{dt} \right)^k = \sum_{k=0}^{\infty} \frac{1}{k!} \left(\Delta t \frac{d}{dt} \right)^k$$

$\hat{H}f = \{f, H\}$

$$e^x = \sum_{k=0}^{\infty} \frac{x^k}{k!} \Rightarrow \boxed{\hat{S} = e^{\Delta t \frac{d}{dt}}} \xrightarrow{\text{Hamiltonian Mechanics}} e^{\Delta t \{\cdot, H\}} \rightarrow e^{\Delta t \hat{H}}$$

Separable Hamiltonian

$$H = F(p_i) + G(q_i) \quad \text{For video games, } H = T(p_i) + V(q_i)$$

$$\hat{T}f = \{f, T\} \quad \hat{V}f = \{f, V\} \Rightarrow \hat{H} = \hat{T} + \hat{V} \Rightarrow f(t_0 + \Delta t) = e^{\Delta t \hat{H}} f(t_0) = e^{\Delta t (\hat{T} + \hat{V})} f(t_0)$$

$$f(t_0 + \Delta t) \approx e^{\Delta t \hat{T}} e^{\Delta t \hat{V}} f(t_0) = e^{\Delta t \hat{T}} e^{\Delta t \hat{V}} \begin{bmatrix} p_n \\ q_n \end{bmatrix}$$

Both $e^{\Delta t \hat{T}}$ and $e^{\Delta t \hat{V}}$ are symplectic/canonical

$$\begin{bmatrix} p_{n+1} \\ q_{n+1} \end{bmatrix} \approx e^{\Delta t \hat{T}} e^{\Delta t \hat{V}} \begin{bmatrix} p_n \\ q_n \end{bmatrix}$$

$$\begin{aligned} &\approx e^{\Delta t \hat{T}} \left(\begin{bmatrix} p_n \\ q_n \end{bmatrix} + \Delta t \left\{ \begin{bmatrix} p_n \\ q_n \end{bmatrix}, V \right\} + \frac{\Delta t^2}{2!} \{\{ \begin{bmatrix} p_n \\ q_n \end{bmatrix}, V \}, V\} + \dots \right) \\ &\approx e^{\Delta t \hat{T}} \left(\begin{bmatrix} p_n \\ q_n \end{bmatrix} + \Delta t \begin{bmatrix} p_n, V \\ q_n, V \end{bmatrix} \right) = e^{\Delta t \hat{T}} \left(\begin{bmatrix} p_n \\ q_n \end{bmatrix} + \Delta t \begin{bmatrix} -\frac{\partial V}{\partial q_n} \\ \frac{\partial V}{\partial p_n} \end{bmatrix} \right) = e^{\Delta t \hat{T}} \begin{bmatrix} p_n + \Delta t F_n \\ q_n \end{bmatrix} = e^{\Delta t \hat{T}} \begin{bmatrix} p_{n+1} \\ q_n \end{bmatrix} \\ &\approx \begin{bmatrix} p_{n+1} \\ q_n \end{bmatrix} + \Delta t \left\{ \begin{bmatrix} p_{n+1} \\ q_n \end{bmatrix}, T \right\} + \dots \approx \begin{bmatrix} p_{n+1} \\ q_n \end{bmatrix} + \Delta t \begin{bmatrix} \frac{\partial T}{\partial p_{n+1}} \\ \frac{\partial T}{\partial q_n} \end{bmatrix} = \begin{bmatrix} p_{n+1} \\ q_n + \Delta t \frac{\partial T}{\partial p_{n+1}} \end{bmatrix} = \begin{bmatrix} p_{n+1} \\ q_{n+1} \end{bmatrix} \end{aligned}$$

Force $= -\frac{\partial V}{\partial q}$

All that implies

$$\begin{bmatrix} p_{n+1} \\ q_{n+1} \end{bmatrix} = \begin{bmatrix} p_n + \Delta t F_n \\ q_n + \Delta t \frac{p_{n+1}}{m} \end{bmatrix} \leftarrow \text{Semi-Implicit Euler v1}$$

$$\begin{bmatrix} p_{n+1} \\ q_{n+1} \end{bmatrix} = \begin{bmatrix} p_n + \Delta t F_{n+1} \\ q_n + \Delta t \frac{p_n}{m} \end{bmatrix} \leftarrow \text{Semi-Implicit Euler v2} \quad \text{where } F_n = F(q_n) \text{ and } F_{n+1} = F(q_{n+1})$$

Difference Between $e^{\Delta t \hat{H}}$ and $e^{\Delta t \hat{T}} e^{\Delta t \hat{V}}$

$$e^{\Delta t \hat{H}} f = f + \Delta t \hat{H} f + \frac{\Delta t^2}{2!} \hat{H}^2 f + \dots = f + \Delta t \hat{H} f + \frac{\Delta t^2}{2!} (\hat{T}^2 + \hat{T} \hat{V} + \hat{V} \hat{T} + \hat{V}^2) f + \dots$$

\hat{T} and \hat{V} commute, so $\hat{T} \hat{V} = \hat{V} \hat{T}$

$$e^{\Delta t \hat{T}} e^{\Delta t \hat{V}} f = e^{\Delta t \hat{T}} (f + \Delta t \hat{V} f + \frac{\Delta t^2}{2!} \hat{V}^2 f + \dots) = e^{\Delta t \hat{T}} f + \Delta t e^{\Delta t \hat{T}} \hat{V} f + \frac{\Delta t^2}{2!} e^{\Delta t \hat{T}} \hat{V}^2 f + \dots$$

$$= (f + \Delta t \hat{T} f + \frac{\Delta t^2}{2!} \hat{T}^2 f + \dots) + \Delta t (\hat{V} f + \Delta t \hat{T} \hat{V} f + \dots) + \frac{\Delta t^2}{2!} (\hat{V}^2 f + \dots)$$

$$= f + \Delta t (\hat{T} + \hat{V}) f + \Delta t^2 (\frac{\hat{T}^2}{2} + \hat{T} \hat{V} + \frac{\hat{V}^2}{2}) f + \dots$$

$$(e^{\Delta t \hat{T}} e^{\Delta t \hat{V}} - e^{\Delta t (\hat{T} + \hat{V})}) f = \left[\cancel{1 + \Delta t (\hat{T} + \hat{V})} + \Delta t^2 (\cancel{\frac{\hat{T}^2}{2} + \hat{T} \hat{V} + \cancel{\frac{\hat{V}^2}{2}}}) + \dots \right] f - \left[\cancel{1 + \Delta t (\hat{T} + \hat{V})} + \Delta t^2 (\cancel{\frac{\hat{T}^2}{2} + \cancel{\frac{\hat{T} \hat{V}}{2}} + \cancel{\frac{\hat{V} \hat{T}}{2}} + \cancel{\frac{\hat{V}^2}{2}}}) + \dots \right] f$$

$$= (\frac{\Delta t^2}{2} (\hat{T} \hat{V} - \hat{V} \hat{T}) + \dots) f = \boxed{(\frac{\Delta t^2}{2} [\hat{T}, \hat{V}] + \dots) f}$$

Where $[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$ is the commutator.

$$\Rightarrow e^{\Delta t \hat{T}} e^{\Delta t \hat{V}} \approx e^{\Delta t (\hat{T} + \hat{V} + \frac{\Delta t}{2} [\hat{T}, \hat{V}] + \dots)} \Rightarrow \boxed{\hat{H}_s \approx \hat{T} + \hat{V} + \frac{\Delta t}{2} [\hat{T}, \hat{V}] + \dots}$$

← Shadow Hamiltonian for Semi-Implicit Euler v1

By a similarly tedious argument or variable substitution,

$$e^{\Delta t \hat{V}} e^{\Delta t \hat{T}} \approx e^{\Delta t (\hat{T} + \hat{V} + \frac{\Delta t}{2} [\hat{V}, \hat{T}] + \dots)} \Rightarrow \boxed{\hat{H}_s \approx \hat{T} + \hat{V} + \frac{\Delta t}{2} [\hat{V}, \hat{T}] + \dots}$$

← Shadow Hamiltonian for Semi-Implicit Euler v2

Higher-Order Symplectic Integrators

Start w/ Shadow Hamiltonian: $\hat{H}_{s1} = \hat{T} + \hat{V} + \frac{\Delta t}{2} [\hat{T}, \hat{V}] + \dots$ $\hat{H}_{s2} = \hat{T} + \hat{V} + \frac{\Delta t}{2} [\hat{V}, \hat{T}] + \dots$

$$[\hat{V}, \hat{T}] = -[\hat{T}, \hat{V}] \Rightarrow \hat{H}_{s1} + \hat{H}_{s2} = 2(\hat{T} + \hat{V} + \dots)$$

Get rid of these terms.

Higher-order terms

Δt^3 and higher

$$Do \underbrace{\left(e^{\Delta t \hat{T}/2} e^{\Delta t \hat{V}/2} \right)}_{\text{Semi-Implicit Euler v1}} \underbrace{\left(e^{\Delta t \hat{V}/2} e^{\Delta t \hat{T}/2} \right)}_{\text{Semi-Implicit Euler v2}} \approx e^{\Delta t \hat{H} + \dots}$$

Verlet Method v1

$$\underbrace{\left(e^{\Delta t \hat{V}/2} e^{\Delta t \hat{T}/2} \right) \left(e^{\Delta t \hat{T}/2} e^{\Delta t \hat{V}/2} \right)}_{\text{Verlet Method v2}} \approx e^{\Delta t \hat{H} + \dots}$$

Verlet Method v1 is better because you only need to calculate the force once.