HMC FT

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Weekly Meeting 2024/10

UNIVERSITY OF MARYLAND

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Implemented code

- Hamiltonian Dynamics
  - Harmonic oscillator
  - Sine potential
- Nambu Dynamics
  - Harmonic oscillator
  - Sine potential

Sampling

- suppose we have 10 values of x: x = (0, 1, 2, 3, 4, ..., 9)
- then we can calculate probability that we want: P(xi) = exp(- H(xi))
- we do the random.uniform sample for 100 attempts, so roughly 10 attempts on each value of x
- the accept rate for xi is A(xi) = P(xi) / Pmax, where Pmax = max{ P(xi) }
- then the number of samples we got on xi is 10 * A(xi) = const * P(xi)
- so we got a set of samples following the probability distribution P(xi)

```python
samples = []
attempts = 0
max_attempts = N * 1000  # To prevent infinite loop

k = 1.0
potential = lambda x: k * (x**2) / 2 # * think about use which potential

potential_min = min(potential(np.linspace(x_bounds[0], x_bounds[1], 1000)))
print(f">>> Potential min: {potential_min}")

while len(samples) < N and attempts < max_attempts:
    # Sample x0 uniformly within bounds
    x_proposal = np.random.uniform(x_bounds[0], x_bounds[1])
    # Compute acceptance probability for x0
    p_x = np.exp(-potential(x_proposal))
    p_x_max = np.exp(-potential_min)  # the minimum of potential corresponds to the maximum of p_x

    if np.random.uniform(0, p_x_max) < p_x:
        # Accept x0
        x0 = x_proposal
        # Sample p0 from Gaussian distribution
        p0 = np.random.normal(0, psigma)
        samples.append((x0, p0))
    attempts += 1

if len(samples) < N:
    raise RuntimeError(f"Could not generate {N} samples within {max_attempts} attempts.")

return samples
```

Check with Analytical results: max displacement

$$< x_{\max} > = \frac{1}{N}\int_{-3}^{3} dx \int dp e^{-(x^2+p^2)/2}\sqrt{x^2+p^2}$$

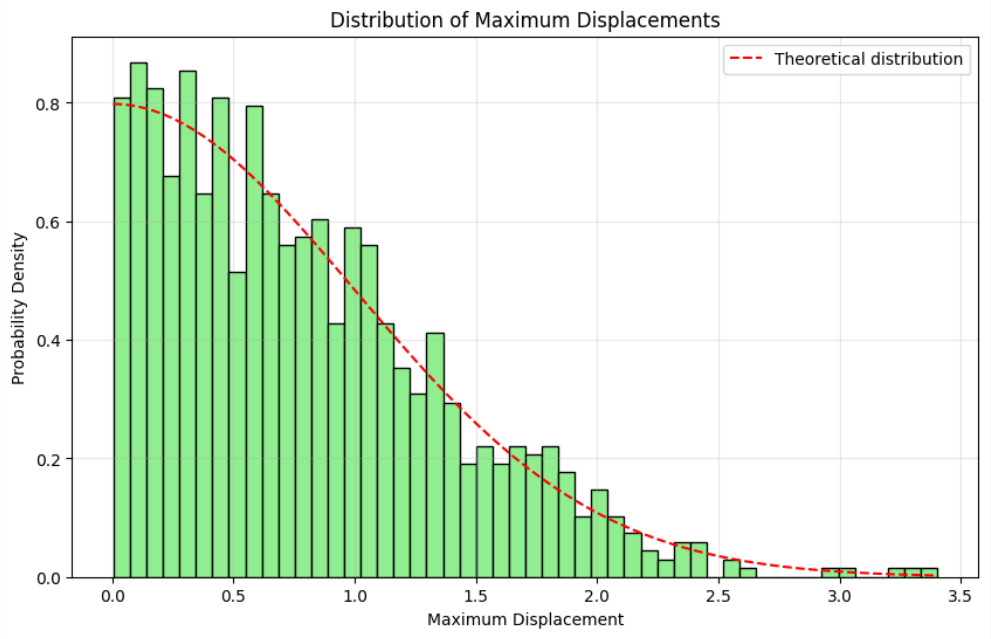
```
In[7]:= maxdisp = NIntegrate[Integrate[Sqrt[x^2 + p^2] * Exp[-(x^2 + p^2) / 2], {p, -∞, ∞}], {x, -3, 3}];
        norm = NIntegrate[Integrate[Exp[-(x^2 + p^2) / 2], {p, -∞, ∞}], {x, -3, 3}];
        maxdisp / norm
Out[9]= 1.24743
```

```
>>> Using Hamiltonian Dynamics:
Loop in samples: 100%|██████████| 1000/1000 [00:02<00:00, 480.46it/s]
Average max displacement: 1.25
```

Check with Analytical results: Pmax

$$P_{max}(x;x_0) = \frac{1}{2}\sqrt{\frac{k}{2\pi}}\int_{|x_0|}^{\infty} ds \frac{s}{\sqrt{s^2-x_0^2}} e^{-(k/2)(s^2-x_0^2)}\delta(x-s) \quad (28)$$

$$= \frac{1}{2}\sqrt{\frac{k}{2\pi}} \frac{x}{\sqrt{x^2-x_0^2}} e^{-(k/2)(x^2-x_0^2)} \quad (29)$$



Hamiltonian v.s. Nambu: Harmonic oscillator

$$H = p^2/2m + kx^2/2$$

$$H = p^2/2m + kx^2/2 + r^2/2m$$

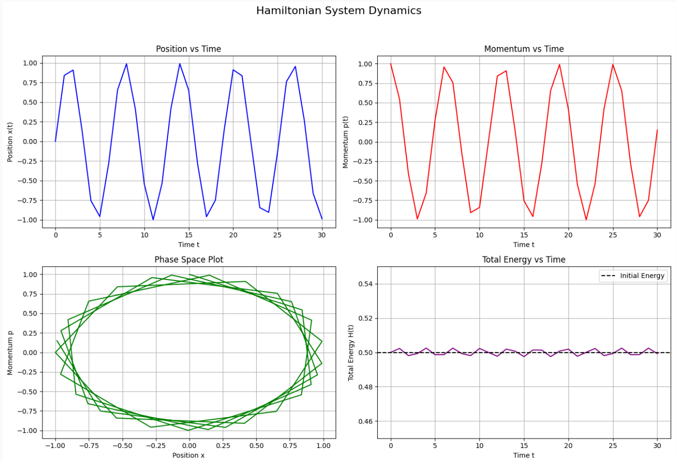
$$G = r^2/2m + kx^2/4$$

$$H - G = p^2/2m + kx^2/4$$

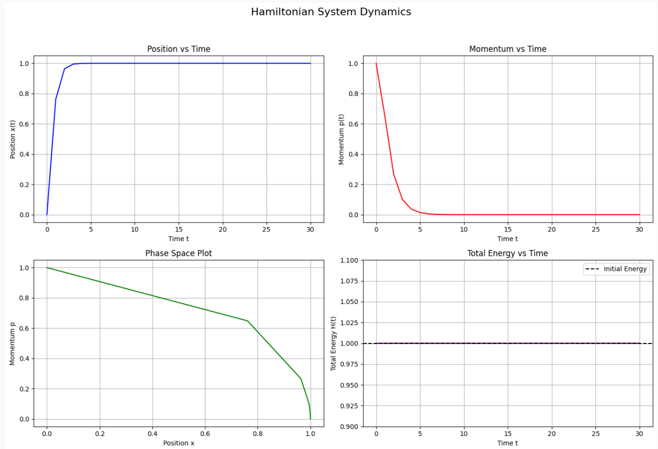
$$k_{\text{Nambu}} = 2k_{\text{Hamilton}} = 2$$

$$\mathrm{p0} = \mathrm{m} = 1$$

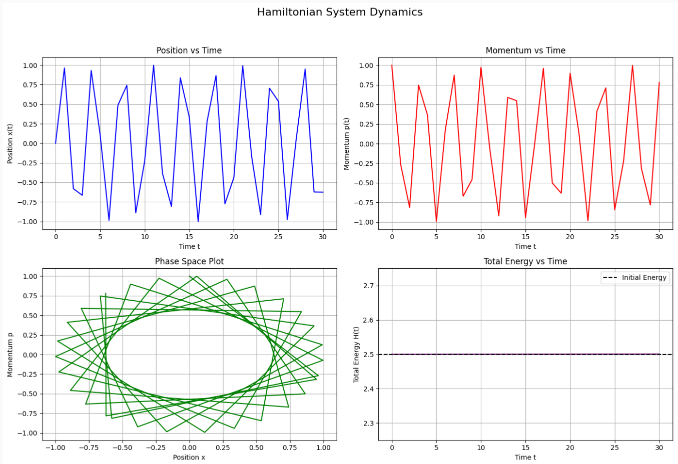
Hamilton



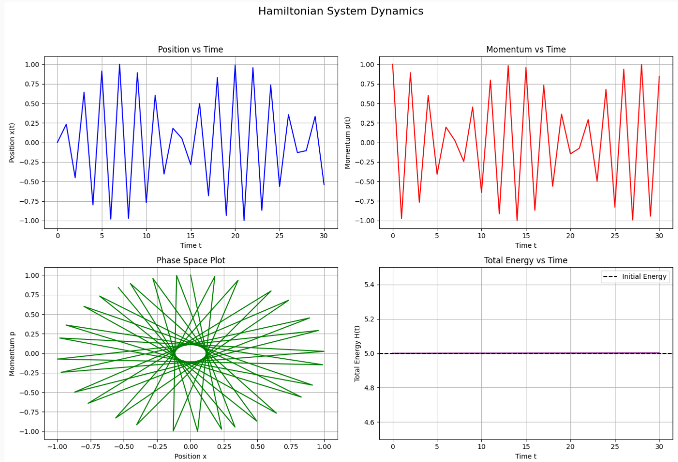
r = 1



r = 2



r = 3



Hamiltonian v.s. Nambu: Harmonic oscillator

$$H = p^2/2m + kx^2/2$$

```
>>> Using Hamiltonian Dynamics:
Loop in samples: 100%|██████████| 1000/1000 [00:02<00:00, 480.46it/s]
Average max displacement: 1.25
```

$$H = p^2/2m + kx^2/2 + r^2/2m$$

$$G = r^2/2m + kx^2/4$$

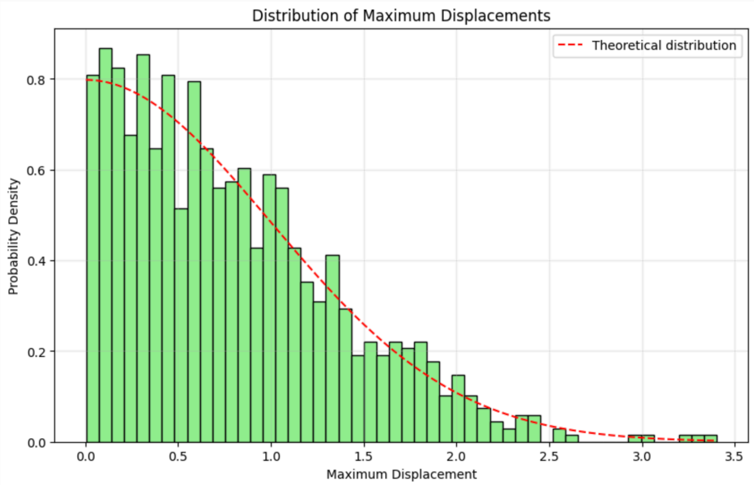
$$H - G = p^2/2m + kx^2/4$$

```
>>> Using Nambu Dynamics:
Loop in samples: 100%|██████████| 1000/1000 [06:31<00:00,  2.55it/s]
Average max displacement: 1.26
```

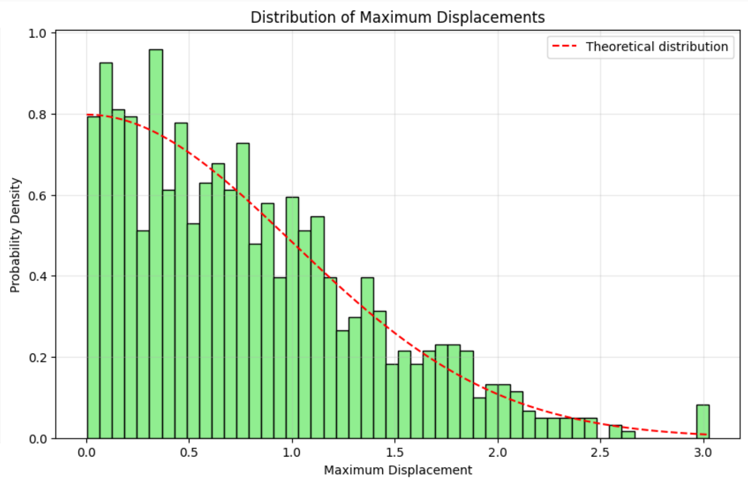
$$k_{\text{Nambu}} = 2k_{\text{Hamilton}} = 2$$

$$\mathrm{p0 = m = 1}$$

Hamiltonian



r = 3



Hamiltonian v.s. Nambu: Harmonic oscillator

$H = p^2/2m + kx^2/2$

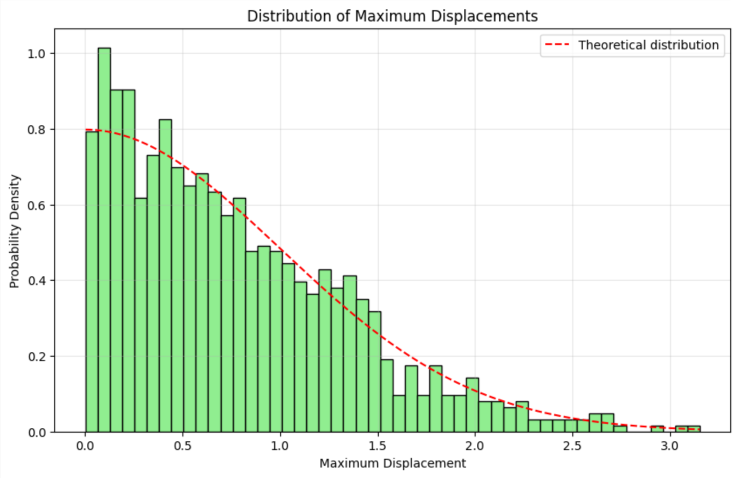
$H = p^2/2m + kx^2/2 + r^2/2m$ Hamiltonian r = 3

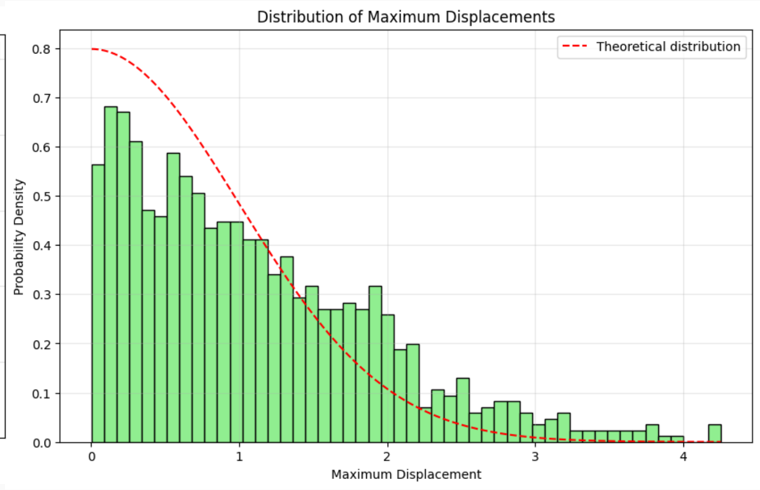
$G = r^2/2m + kx^2/4$

$H - G = p^2/2m + kx^2/4$

$k_{\text{Nambu}} = k_{\text{Hamilton}} = 1$

p0 = m = 1





Hamiltonian v.s. Nambu: Sine

$$H = p^2/2m + k\sin(x)$$

$$H = p^2/2m + k\sin(x) + r^2/2m$$

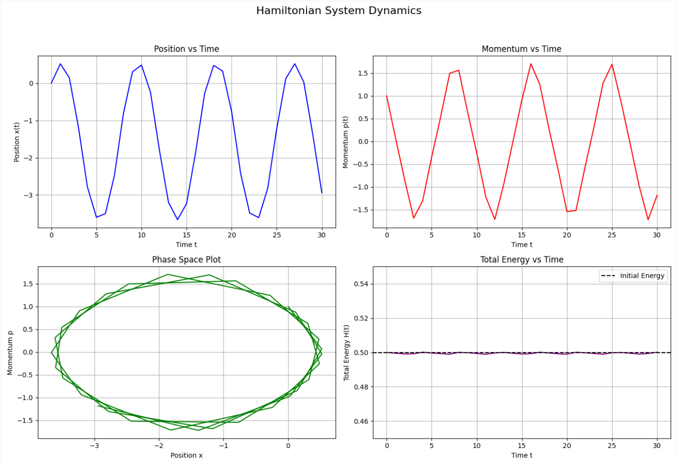
$$G = r^2/2m + k\sin(x)/2$$

$$H - G = p^2/2m + k\sin(x)/2$$

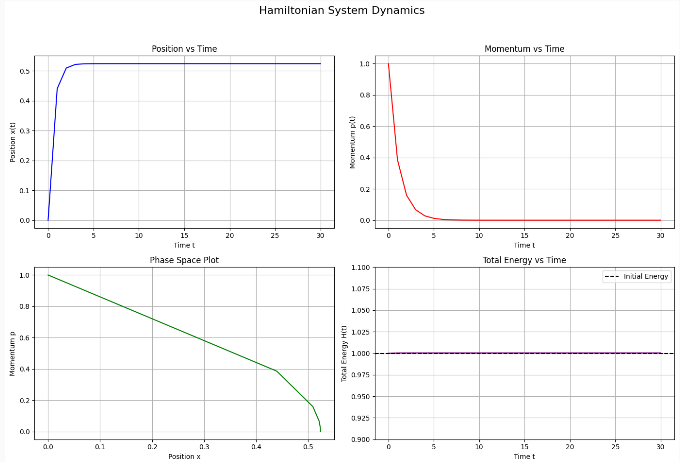
$$k_{\text{Nambu}} = 2k_{\text{Hamilton}} = 2$$

p0 = m = 1

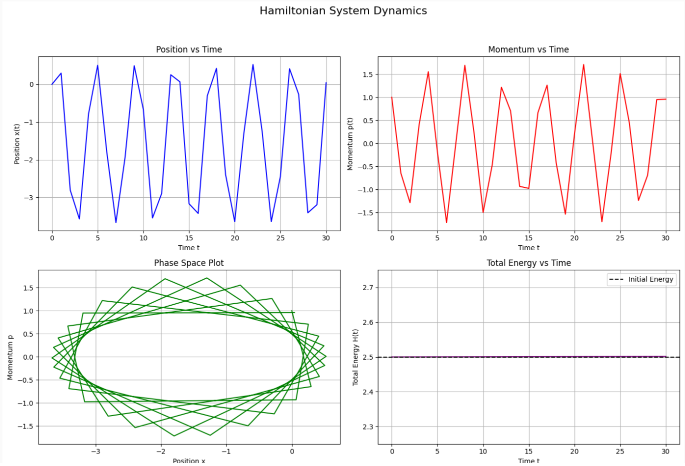
Hamilton



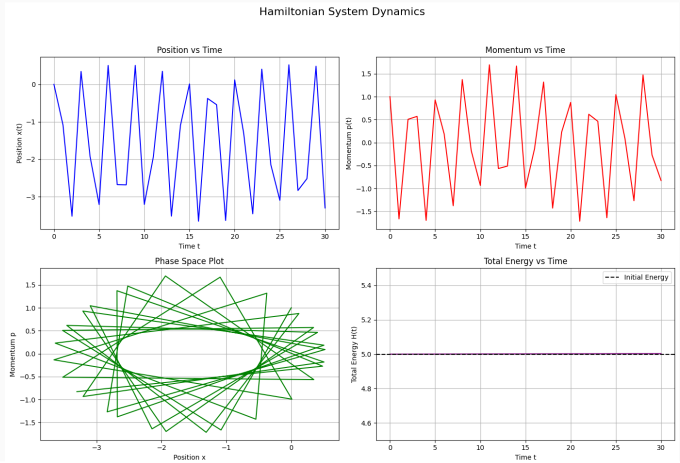
r = 1



r = 2



r = 3



Hamiltonian v.s. Nambu: Sine

$$H = p^2/2m + k\sin(x)$$

$$H = p^2/2m + k\sin(x) + r^2/2m$$

$$G = r^2/2m + k\sin(x)/2$$

$$H - G = p^2/2m + k\sin(x)/2$$

$$k_{\text{Nambu}} = 2k_{\text{Hamilton}} = 2$$

p0 = m = 1

```
>>> Using Hamiltonian Dynamics:
Loop in samples:  10%|█          | 48/500 [00:00<00:07, 57.29it/s]
Loop in samples: 100%|███████████| 500/500 [00:08<00:00, 57.35it/s]

>>> Average number of times crossing the potential maxima: 1.14
```

```
>>> Using Nambu Dynamics:
Loop in samples: 100%|███████████| 500/500 [18:44<00:00,  2.25s/it]

>>> Average number of times crossing the potential maxima: 1.41
```