Accelerated Tempering Dynamics in HMC Simulations of Lattice Field Theory

Jack Frankland

University of Edinburgh

April 2, 2018

Introduction

- What are we doing?
  - Calculating properties of Quantum Mechanical Systems.

Introduction

- What are we doing?
  - Calculating properties of Quantum Mechanical Systems.
- How are we doing it?
  - Using a MCMC (Markov chain Monte Carlo) method - Hybrid Monte Carlo [1].

Introduction

- What are we doing?
  - Calculating properties of Quantum Mechanical Systems.
- How are we doing it?
  - Using a MCMC (Markov chain Monte Carlo) method - Hybrid Monte Carlo [1].
- What results have we got?
  - Successfully reproduced theoretical results for harmonic and anharmonic oscillators.

Introduction

- What are we doing?
  - Calculating properties of Quantum Mechanical Systems.
- How are we doing it?
  - Using a MCMC (Markov chain Monte Carlo) method - Hybrid Monte Carlo [1].
- What results have we got?
  - Successfully reproduced theoretical results for harmonic and anharmonic oscillators.
- What is the aim?
  - To improve the algorithm using *tempering* dynamics - solve problem of isolated modes.

Introduction

- What are we doing?
  - Calculating properties of Quantum Mechanical Systems.
- How are we doing it?
  - Using a MCMC (Markov chain Monte Carlo) method - Hybrid Monte Carlo [1].
- What results have we got?
  - Successfully reproduced theoretical results for harmonic and anharmonic oscillators.
- What is the aim?
  - To improve the algorithm using *tempering* dynamics - solve problem of isolated modes.
- Why are we doing it?
  - Can be used for calculations in lattice field theory[2].

The Path Integral

Transition Amplitude

$$\langle x_b, t_b | x_a, t_a \rangle = \int_{x_a}^{x_b} \mathcal{D}x \exp\left(iS_M\left[x\left(t\right)\right]\right)$$

The Path Integral

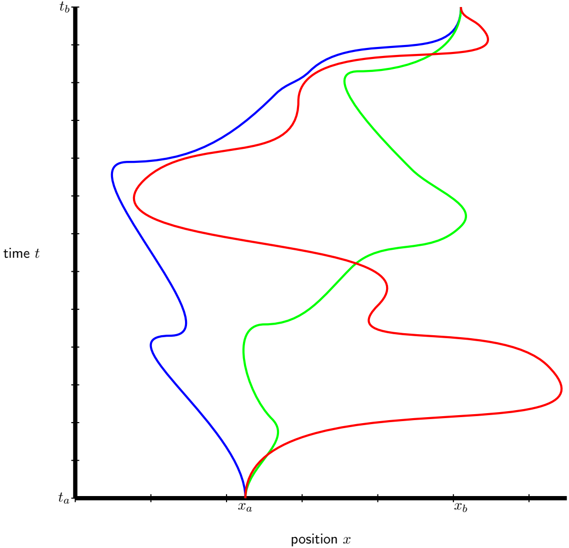
Transition Amplitude

$$\langle x_b, t_b | x_a, t_a \rangle = \int_{x_a}^{x_b} \mathcal{D}x \exp\left(i S_M \left[x\left(t\right)\right]\right)$$

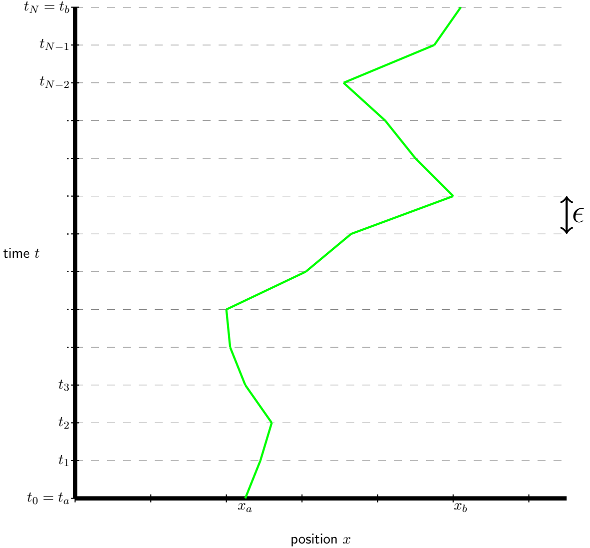
Minkowski Action

$$S_M \left[x\left(t\right)\right] = \int_{t_a}^{t_b} dt \left[\frac{1}{2} m \left(\frac{dx}{dt}\right)^2 - V\left(x\right)\right]$$

The Path Integral



Discrete Time Lattice



Discrete Time Lattice

Configuration

$$\boldsymbol{x} = (x_0, x_1, \ldots, x_{N-1})$$

$$x_i = x\,(t_i)$$

Discrete Time Lattice

Configuration

$$\boldsymbol{x} = (x_0, x_1, \ldots, x_{N-1})$$

$$x_i = x(t_i)$$

Wick Rotation

$$\tau = it$$

Discrete Time Lattice

Configuration

$$\boldsymbol{x} = (x_0, x_1, \ldots, x_{N-1})$$

$$x_i = x\,(t_i)$$

Wick Rotation

$$\tau = it$$

$$a = i\epsilon$$

Connecting to Statistical Mechanics

Discrete Euclidean Path Integral

$$Z \sim \int_{-\infty}^{\infty} \prod_{j=0}^{N-1} dx_j \exp\left(-S_E\left(\boldsymbol{x}\right)\right)$$

Connecting to Statistical Mechanics

Quantum Expectation Values

$$
\begin{aligned}
\langle 0 | \hat{A} | 0 \rangle &= \frac{\int_{-\infty}^{+\infty} \prod_{i=0}^{N-1} dx_i A\left(x_0, \ldots, x_{N-1}\right) \exp\left(-S_E\left(\boldsymbol{x}\right)\right)}{\int_{-\infty}^{+\infty} \prod_{i=0}^{N-1} dx_i \exp\left(-S_E\left(\boldsymbol{x}\right)\right)} \\
&= \langle A \rangle
\end{aligned}
$$

Monte Carlo

Expectation Value

$$\langle A \rangle = \int \prod_{i=0}^{N-1} dx_i p\left(\boldsymbol{x}\right) A\left(\boldsymbol{x}\right)$$

Monte Carlo

Expectation Value

$$\langle A \rangle = \int \prod_{i=0}^{N-1} dx_i p\left(\boldsymbol{x}\right) A\left(\boldsymbol{x}\right)$$

Monte Carlo Estimate

$$\langle A \rangle = \frac{1}{M} \sum_{n=1}^{M} A\left(\boldsymbol{x}_n\right)$$

Monte Carlo

Monte Carlo Estimate

$$\langle A \rangle = \frac{1}{M} \sum_{n=1}^{M} A\left(\boldsymbol{x}_n\right)$$

Boltzmann Distribution

$$p\left(\boldsymbol{x}\right) = \frac{1}{Z} \exp\left(-S_E\left(\boldsymbol{x}\right)\right)$$

Hybrid Monte Carlo Algorithm - The Set Up

Fictitious Momenta

$$\boldsymbol{p} = (p_0, p_1, \ldots, p_{N-1})$$

Hybrid Monte Carlo Algorithm - The Set Up

Fictitious Momenta

$$\boldsymbol{p} = (p_0, p_1, \ldots, p_{N-1})$$

HMC Hamiltonian

$$H_{HMC}(\boldsymbol{x}, \boldsymbol{p}) := \sum_{i=0}^{N-1} \frac{p_i^2}{2} + S_E(\boldsymbol{x})$$

The Hybrid Monte Carlo Algorithm

HMC Algorithm

0. Provide initial configuration x.

The Hybrid Monte Carlo Algorithm

HMC Algorithm

0. Provide initial configuration $\boldsymbol{x}$.
1. Generate $\boldsymbol{p}$ from $\mathcal{N}\left(\mathbf{0}, \mathbb{I}\right)$.

The Hybrid Monte Carlo Algorithm

HMC Algorithm

0. Provide initial configuration $\boldsymbol{x}$.
1. Generate $\boldsymbol{p}$ from $\mathcal{N}\left(\mathbf{0}, \mathbb{I}\right)$.
2. Evolve $(\boldsymbol{x}, \boldsymbol{p})$ using Hamilton's equation's to a final state $(\boldsymbol{x}', \boldsymbol{p}')$ then negate the momenta $(\boldsymbol{x}', -\boldsymbol{p}')$.

The Hybrid Monte Carlo Algorithm

HMC Algorithm

0. Provide initial configuration $\boldsymbol{x}$.
1. Generate $\boldsymbol{p}$ from $\mathcal{N}(\mathbf{0}, \mathbb{I})$.
2. Evolve $(\boldsymbol{x}, \boldsymbol{p})$ using Hamilton's equation's to a final state $(\boldsymbol{x}', \boldsymbol{p}')$ then negate the momenta $(\boldsymbol{x}', -\boldsymbol{p}')$.
3. Accept configuration $\boldsymbol{x}$ with probability $\min\left[1, \exp\left(-H_{HMC}\left(\boldsymbol{x}', \boldsymbol{p}'\right) + H_{HMC}\left(\boldsymbol{x}, \boldsymbol{p}\right)\right)\right]$ (Metropolis update).

The Hybrid Monte Carlo Algorithm

HMC Algorithm

0. Provide initial configuration $\boldsymbol{x}$.
1. Generate $\boldsymbol{p}$ from $\mathcal{N}(\mathbf{0}, \mathbb{I})$.
2. Evolve $(\boldsymbol{x}, \boldsymbol{p})$ using Hamilton's equation's to a final state $(\boldsymbol{x}', \boldsymbol{p}')$ then negate the momenta $(\boldsymbol{x}', -\boldsymbol{p}')$.
3. Accept configuration $\boldsymbol{x}$ with probability $\min\left[1, \exp\left(-H_{HMC}(\boldsymbol{x}', \boldsymbol{p}') + H_{HMC}(\boldsymbol{x}, \boldsymbol{p})\right)\right]$ (Metropolis update).
4. Return to step 1.

Harmonic Oscillator

The potential

$$V\left(x\right) = \frac{\mu^2}{2} x^2$$

Harmonic Oscillator

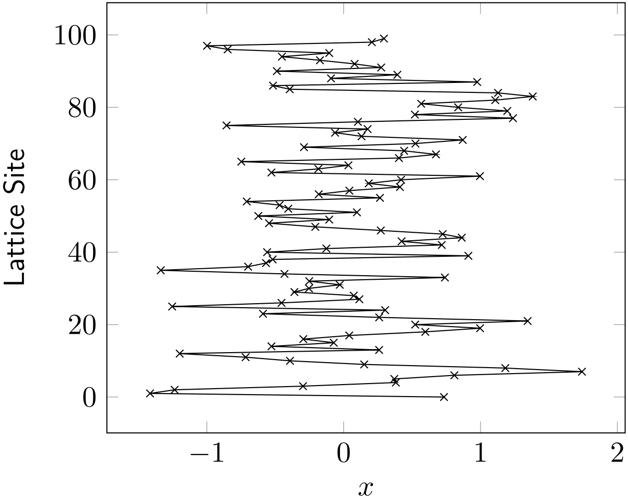
The potential

$$V\left(x\right) = \frac{\mu^2}{2} x^2$$

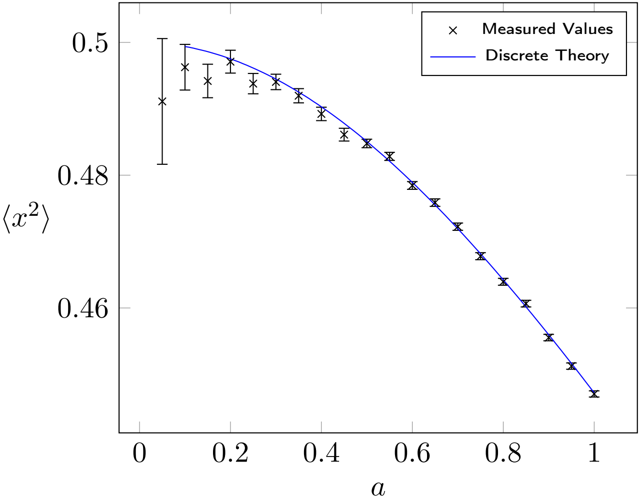
The HMC Hamiltonian

$$H_{HMC}\left(\boldsymbol{x}, \boldsymbol{p}\right) = \sum_{i=0}^{N-1} \frac{p_i^2}{2} + \sum_{i=0}^{N-1} a \left[\frac{1}{2} m \left(\frac{x_{i+1} - x_i}{a} \right)^2 + \frac{1}{2} \mu^2 x_i^2 \right]$$

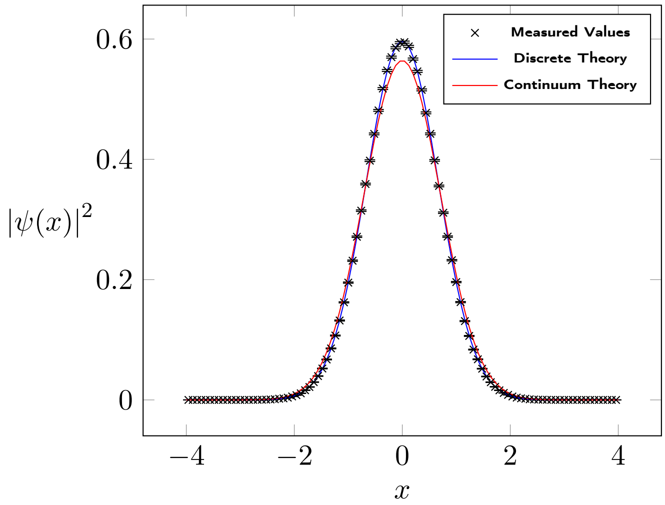
Harmonic Oscillator Typical Configuration



Harmonic Oscillator Expectation Values



Harmonic Oscillator Ground State Probability Density



Anharmonic Oscillator

The potential

$$V\left(x\right) = \lambda\left(x^2 - f^2\right)^2$$

Anharmonic Oscillator

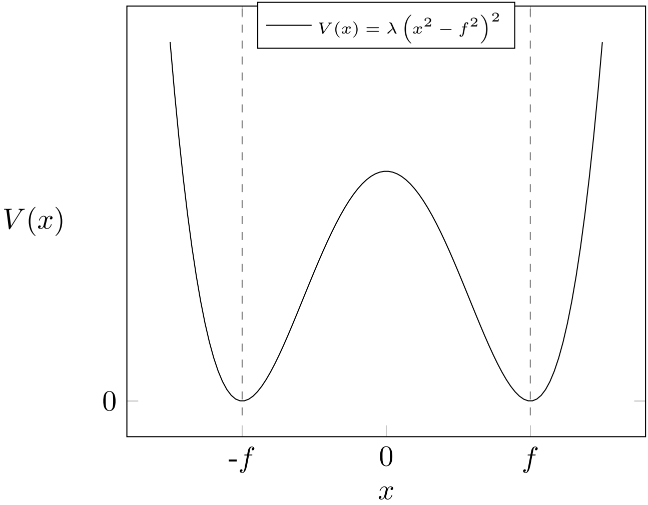
The potential

$$V\left(x\right)=\lambda\left(x^{2}-f^{2}\right)^{2}$$

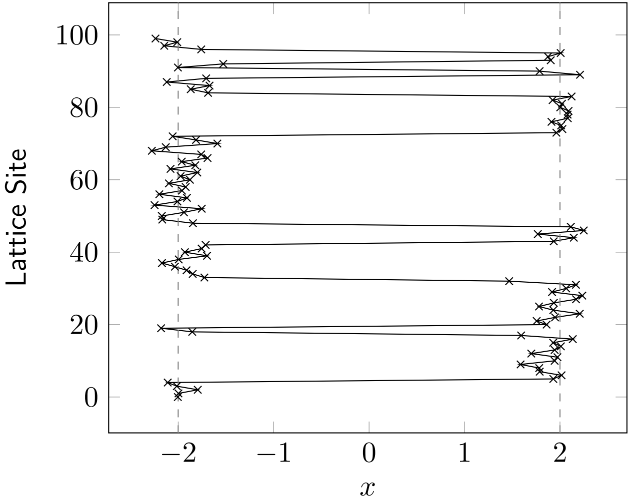
The HMC Hamiltonian

$$H_{HMC}\left(\boldsymbol{x},\boldsymbol{p}\right)=\sum_{i=0}^{N-1}\frac{p_i^2}{2}+\sum_{i=0}^{N-1}a\left[\frac{1}{2}m\left(\frac{x_{i+1}-x_i}{a}\right)^{2}+\lambda\left(x_i^2-f^2\right)^{2}\right]$$

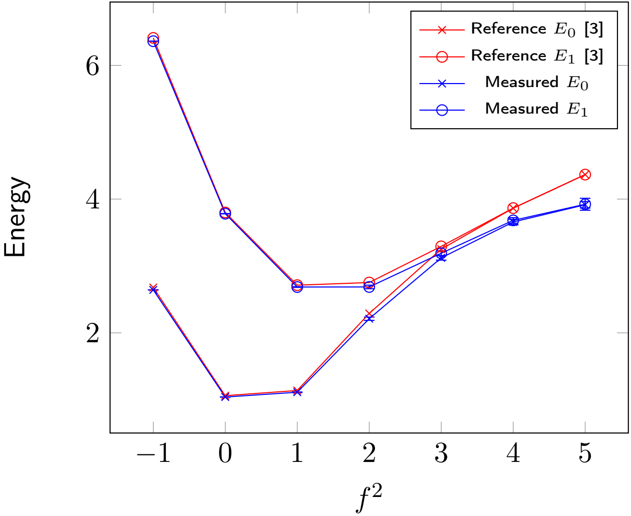
Anharmonic Oscillator



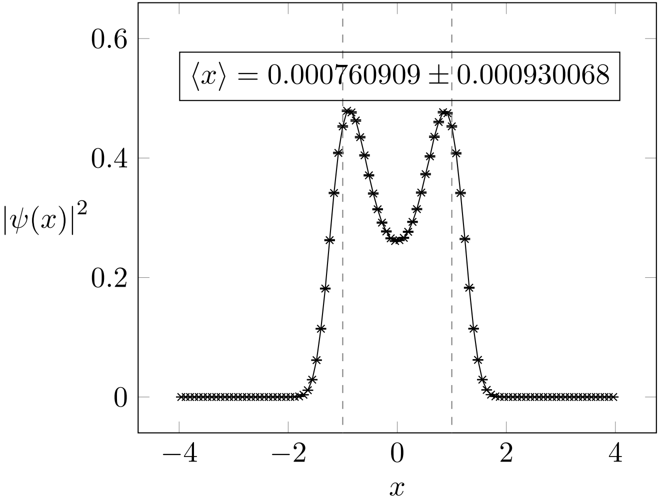
Anharmonic Oscillator Typical Configuration



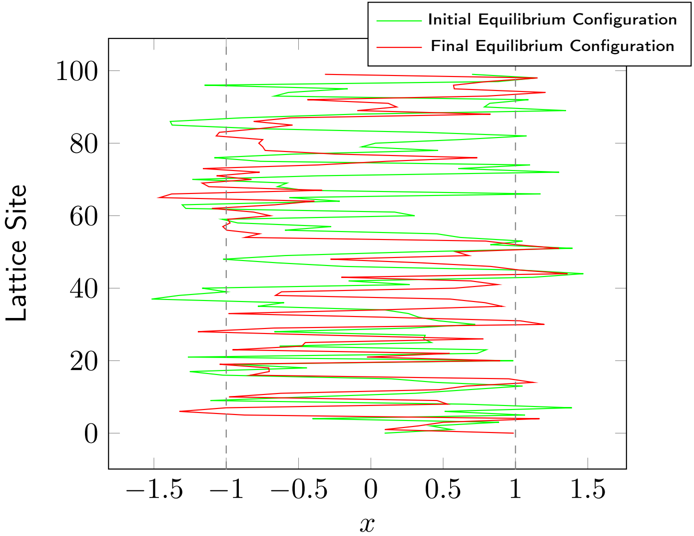
Anharmonic Oscillator Expectation Values



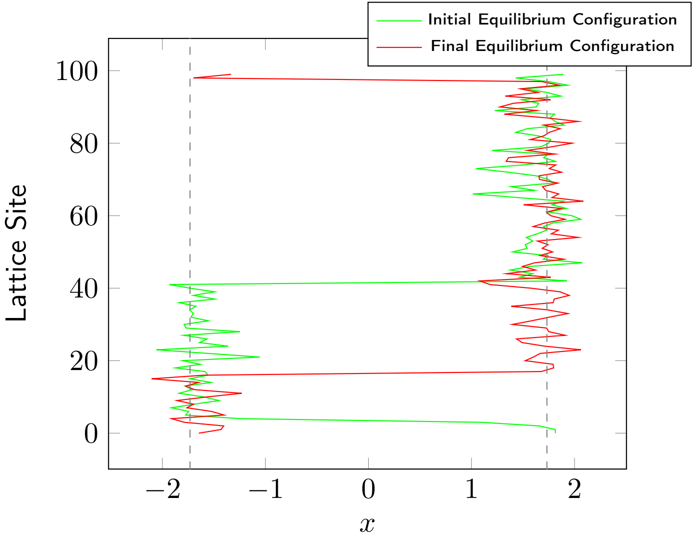
Anharmonic Oscillator Ground State Density Function



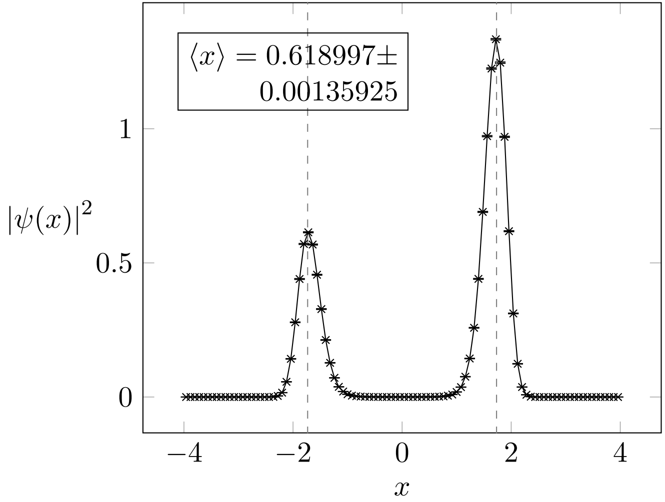
Isolated Modes $f = 1$



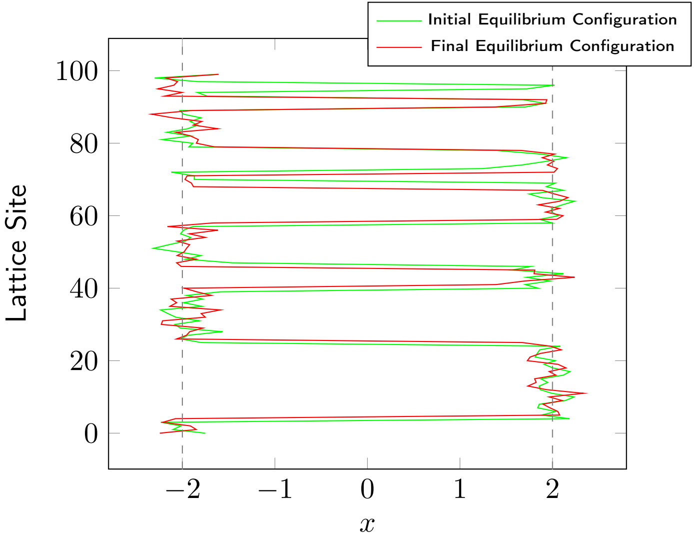
Isolated Modes $f = \sqrt{3}$



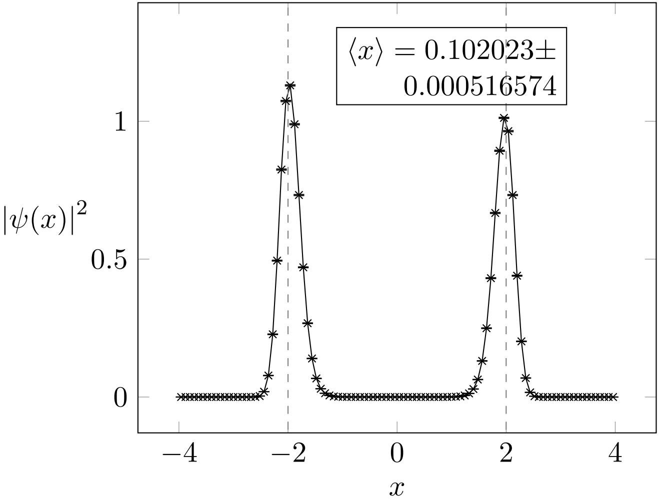
Isolated Modes $f = \sqrt{3}$



Isolated Modes $f = 2$



Isolated Modes $f = 2$



Tempering

- What is tempering?
  - Method to sample from more diffuse probability distribution.

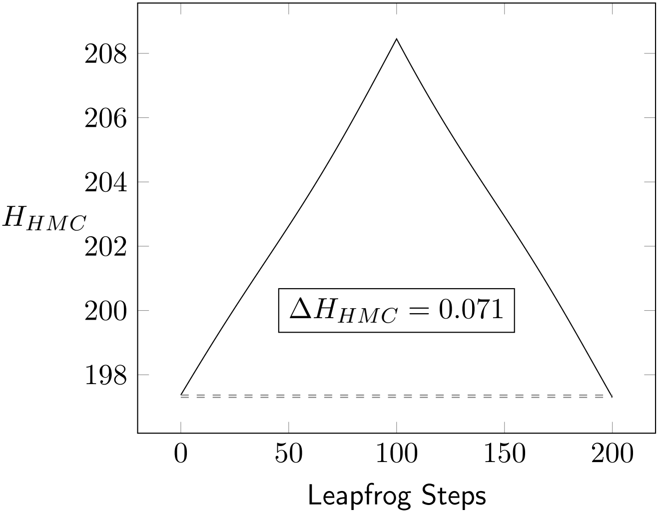
Tempering

- What is tempering?
  - Method to sample from more diffuse probability distribution.
- How is it incorporated into HMC?
  - Multiply and divide momentum variables during the numerical integration of Hamilton's equations by a tempering parameter α [4].

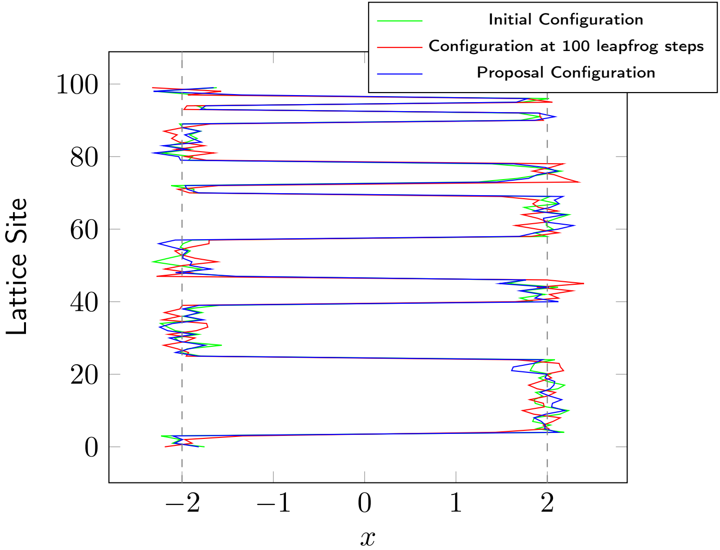
Tempering

- What is tempering?
  - Method to sample from more diffuse probability distribution.
- How is it incorporated into HMC?
  - Multiply and divide momentum variables during the numerical integration of Hamilton's equations by a tempering parameter α [4].
- What results would we expect?
  - Better estimates on expectation values and less correlation between configurations.

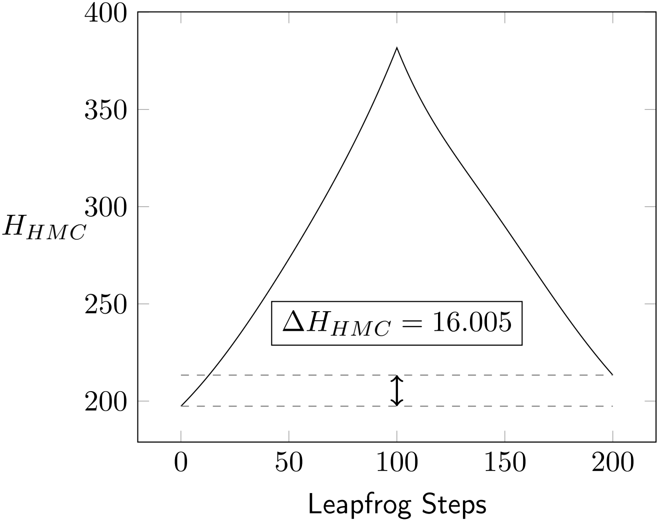
Molecular Dynamics Hamiltonian Evolution $\alpha = 1.001, f = 2$



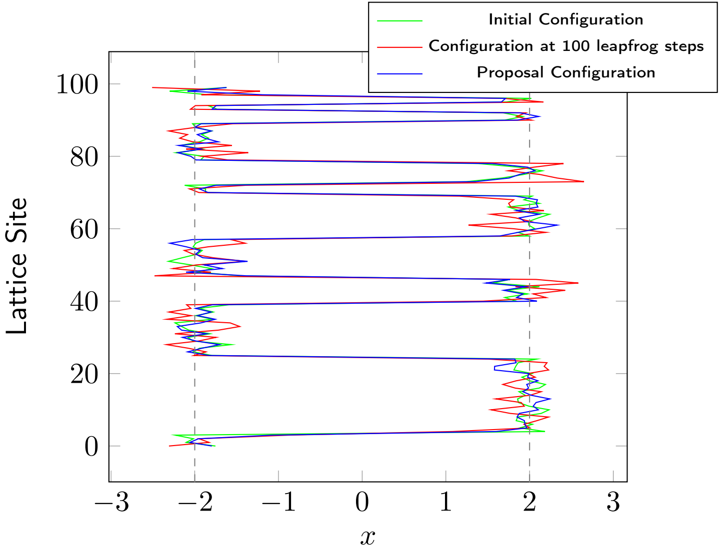
Molecular Dynamics Configuration Evolution $\alpha = 1.001, f = 2$



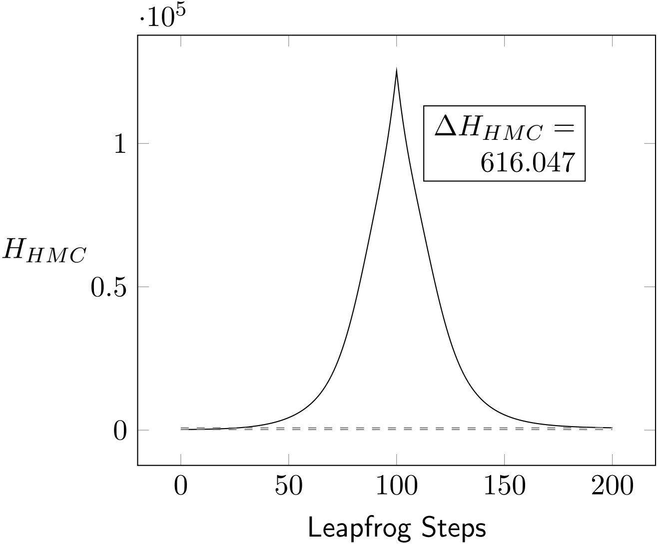
Molecular Dynamics Hamiltonian Evolution $\alpha = 1.01, f = 2$



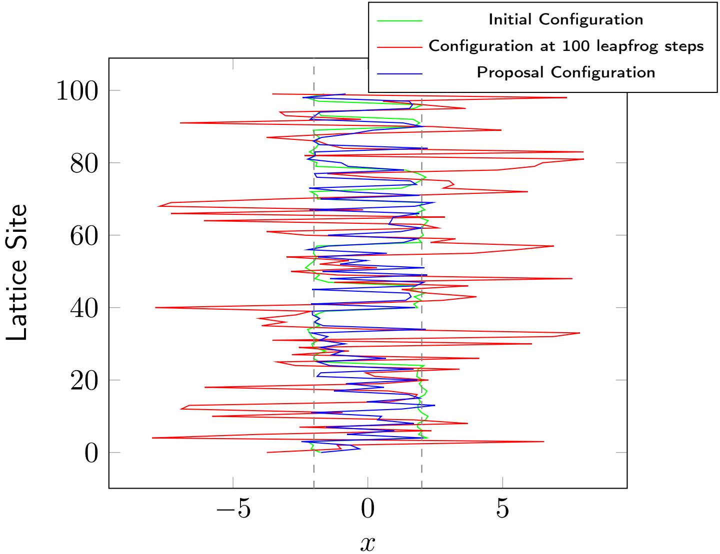
Molecular Dynamics Configuration Evolution $\alpha = 1.01, f = 2$



Molecular Dynamics Hamiltonian Evolution $\alpha = 1.05, f = 2$



Molecular Dynamics Configuration Evolution $\alpha = 1.05, f = 2$



Conclusion

- Did it work?
  - Successfully reproduced results using HMC method.

Conclusion

- Did it work?
  - Successfully reproduced results using HMC method.
- What about tempering?
  - Hamiltonian too high at end of molecular dynamics for proposal to be accepted in cases where tunnelling occurred.

Conclusion

- Did it work?
  - Successfully reproduced results using HMC method.
- What about tempering?
  - Hamiltonian too high at end of molecular dynamics for proposal to be accepted in cases where tunnelling occurred.
- Suggestions for future work?
  - Experiment with the possibility of tempering only a few lattice variables.

References I

Simon Duane, A.d. Kennedy, Brian J. Pendleton, and Duncan Roweth.
Hybrid monte carlo.
Physics Letters B, 195(2):216–222, 1987.

Wolfgang Bietenholz.
Hadron physics from lattice qcd.
International Journal of Modern Physics E, 25(07):1642008, 2016.

R. Blankenbecler, T. Degrand, and R. L. Sugar.
Moment method for eigenvalues and expectation values.
Physical Review D, 21(4):1055–1061, 1980.

References II

Radford Neal.
Mcmc using hamiltonian dynamics.
Chapman & Hall/CRC Handbooks of Modern Statistical Methods Handbook of Markov Chain Monte Carlo, Oct 2011.

Leapfrog Integration

Hamiltonian

$$H(\boldsymbol{q}, \boldsymbol{p}) = U(\boldsymbol{q}) + K(\boldsymbol{p})$$

Leapfrog Integration

Hamiltonian

$$H(\boldsymbol{q}, \boldsymbol{p}) = U(\boldsymbol{q}) + K(\boldsymbol{p})$$

Leapfrog Equations

$$p_i(t + \epsilon/2) = p_i(t) - \epsilon/2 \frac{\partial U}{\partial q_i}(\boldsymbol{q}(t))$$

$$q_i(t + \epsilon) = q_i(t) + \epsilon \frac{\partial K}{\partial p_i}(\boldsymbol{p}(t + \epsilon/2))$$

$$p_i(t + \epsilon) = p_i(t + \epsilon/2) - \epsilon/2 \frac{\partial U}{\partial q_i}(\boldsymbol{q}(t + \epsilon))$$

Leapfrog Integration

Tempered Leapfrog Equations First Half Trajectory

$$p_i\left(t+\epsilon/2\right)=\sqrt{\alpha}p_i\left(t\right)-\epsilon/2\frac{\partial U}{\partial q_i}\left(\boldsymbol{q}\left(t\right)\right)$$

$$q_i\left(t+\epsilon\right)=q_i\left(t\right)+\epsilon\frac{\partial K}{\partial p_i}\left(\boldsymbol{p}\left(t+\epsilon/2\right)\right)$$

$$p_i\left(t+\epsilon\right)=\sqrt{\alpha}\left(p_i\left(t+\epsilon/2\right)-\epsilon/2\frac{\partial U}{\partial q_i}\left(\boldsymbol{q}\left(t+\epsilon\right)\right)\right)$$

Leapfrog Integration

Tempered Leapfrog Equations Second Half Trajectory

$$p_i\left(t+\epsilon/2\right) = \frac{1}{\sqrt{\alpha}} p_i\left(t\right) - \epsilon/2 \frac{\partial U}{\partial q_i}\left(\boldsymbol{q}\left(t\right)\right)$$

$$q_i\left(t+\epsilon\right) = q_i\left(t\right) + \epsilon \frac{\partial K}{\partial p_i}\left(\boldsymbol{p}\left(t+\epsilon/2\right)\right)$$

$$p_i\left(t+\epsilon\right) = \frac{1}{\sqrt{\alpha}}\left(p_i\left(t+\epsilon/2\right) - \epsilon/2 \frac{\partial U}{\partial q_i}\left(\boldsymbol{q}\left(t+\epsilon\right)\right)\right)$$