

Accelerated Tempering Dynamics in HMC Simulations of Lattice Field Theory

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Introduction

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 - ▶ Calculating properties of Quantum Mechanical Systems.

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 - ▶ Successfully reproduced theoretical results for harmonic and anharmonic oscillators.

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 - ▶ 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

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

Probability density of $(x_b, t_b) \rightarrow (x_a, t_a)$.

Integral over all paths between (x_b, t_b) and (x_a, t_a) .

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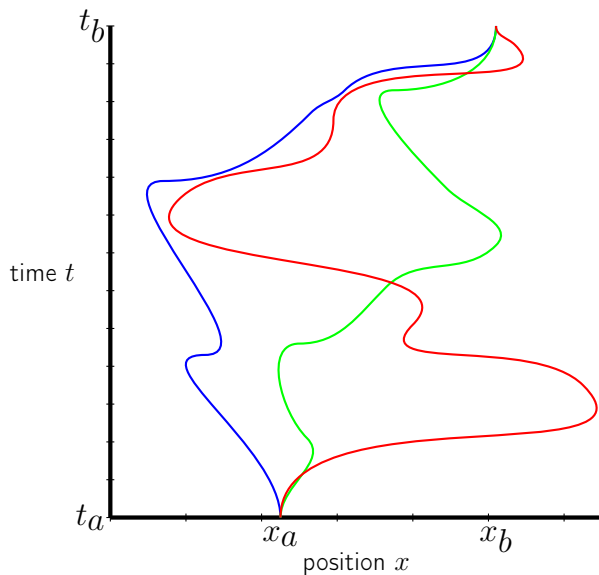
Probability density of $(x_b, t_b) \rightarrow (x_a, t_a)$.

Integral over all paths between (x_b, t_b) and (x_a, t_a) .

Minkowski Action

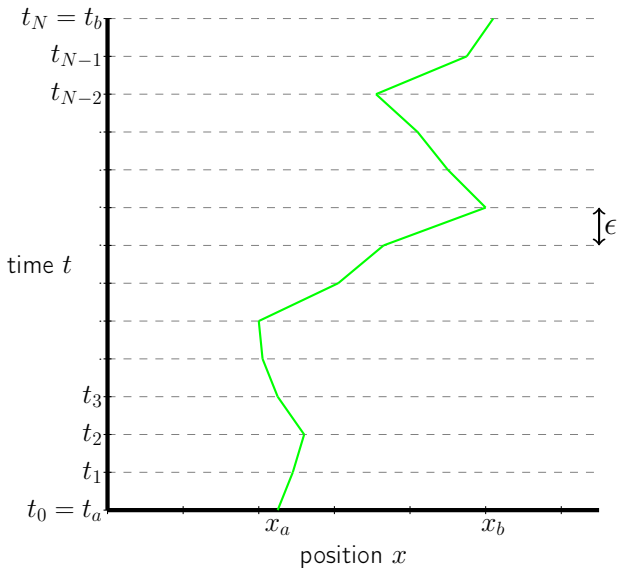
$$S_M[x(t)] = \int_{t_a}^{t_b} dt \left[\frac{1}{2} m \left(\frac{dx}{dt} \right)^2 - V(x) \right]$$

The Path Integral



Three possible paths from (x_a, t_a) to (x_b, t_b) .

Discrete Time Lattice



Discretising time and a path from (x_a, t_a) to (x_b, t_b) onto a lattice of time spacing ϵ .

Discrete Time Lattice

Configuration

Specific path through lattice, each lattice variable specified:

$$\mathbf{x} = (x_0, x_1, \dots, x_{N-1})$$

$$x_i = x(t_i)$$

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Wick Rotation

Substitution for imaginary time:

$$\tau = it$$

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Wick Rotation

Substitution for imaginary time:

$$\tau = it$$

Rotate lattice through complex plane into imaginary time of lattice spacing:

$$a = i\epsilon$$

Connecting to Statistical Mechanics

Discrete Euclidean Path Integral

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

Partition function of statistical mechanical system if
 $H(\mathbf{x}) = S_E(\mathbf{x})$.

Connecting to Statistical Mechanics

Quantum Expectation Values

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

Ground state energy corresponds to statistical expectation of function A on lattice.

Monte Carlo

Expectation Value

Integrals cannot be computed analytically:

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

Monte Carlo

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Monte Carlo Estimate

Approximate integral as sample mean on equilibrium lattice configurations \mathbf{x}_n :

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

Monte Carlo

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Boltzmann Distribution

Generate the configurations \boldsymbol{x}_n according to canonical distribution:

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

Hybrid Monte Carlo Algorithm - The Set Up

Fictitious Momenta

Introduce fictitious momentum variable to go with each lattice variable:

$$\mathbf{p} = (p_0, p_1, \dots, p_{N-1})$$

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HMC Hamiltonian

Hamiltonian for the joint canonical but separable distribution of (\mathbf{x}, \mathbf{p}) :

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

The Hybrid Monte Carlo Algorithm

HMC Algorithm

0. Provide initial configuration x .

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3. Accept configuration \mathbf{x} with probability $\min[1, \exp(-H_{HMC}(\mathbf{x}', \mathbf{p}') + H_{HMC}(\mathbf{x}, \mathbf{p}))]$ (Metropolis update).

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4. Return to step 1.

Harmonic Oscillator

The potential

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

Harmonic Oscillator

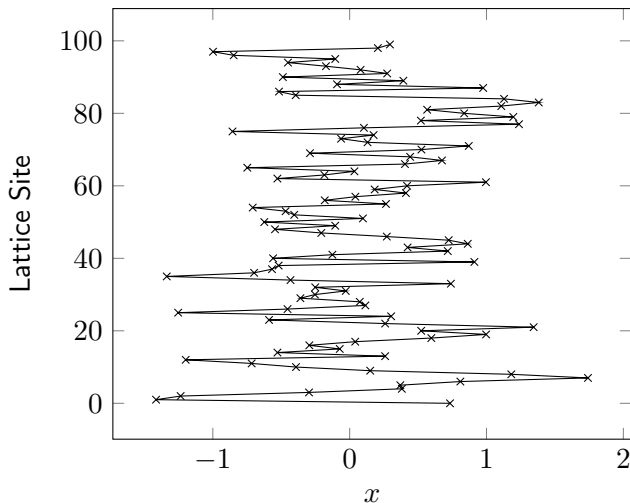
The potential

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The HMC Hamiltonian

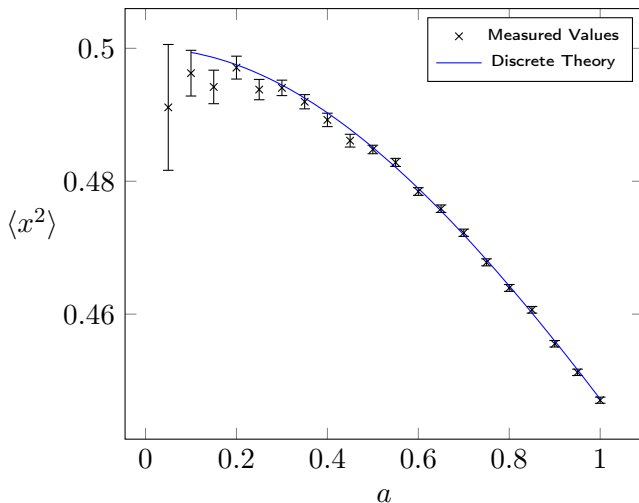
$$H_{HMC}(\mathbf{x}, \mathbf{p}) = \sum_{i=0}^{N-1} \frac{p_i^2}{2} + \sum_{i=0}^{N-1} a \left[\frac{1}{2} m \left(\frac{x_{i+1} - x_i}{a} \right)^2 + \frac{1}{2} \mu^2 x_i^2 \right]$$

Harmonic Oscillator Typical Configuration



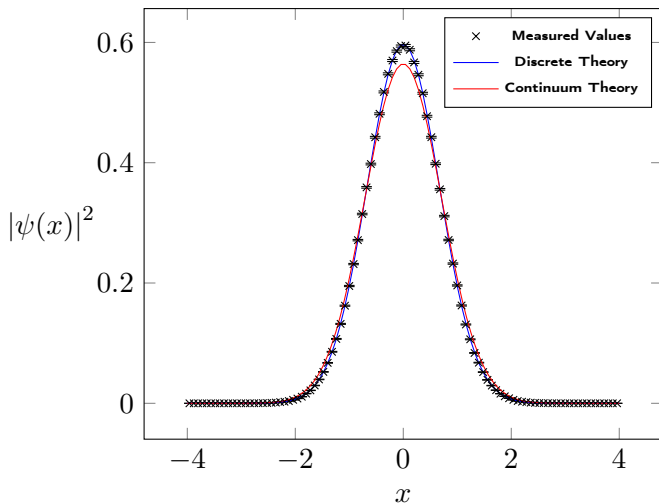
Typical equilibrium configuration on 100 site lattice at spacing $a = 1$ with harmonic potential $\mu = 1$.

Harmonic Oscillator Expectation Values



Mean position squared for a range of finite lattice spacings on a 100 site lattice with harmonic potential $\mu = 1$.

Harmonic Oscillator Ground State Probability Density



Ground state probability density function for 100 site lattice at spacing $a = 1$ for harmonic potential $\mu = 1$.

Anharmonic Oscillator

The potential

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

Anharmonic Oscillator

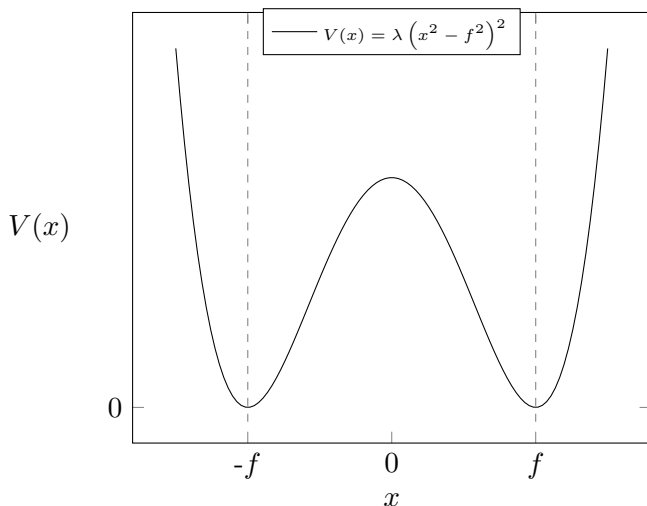
The potential

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The HMC Hamiltonian

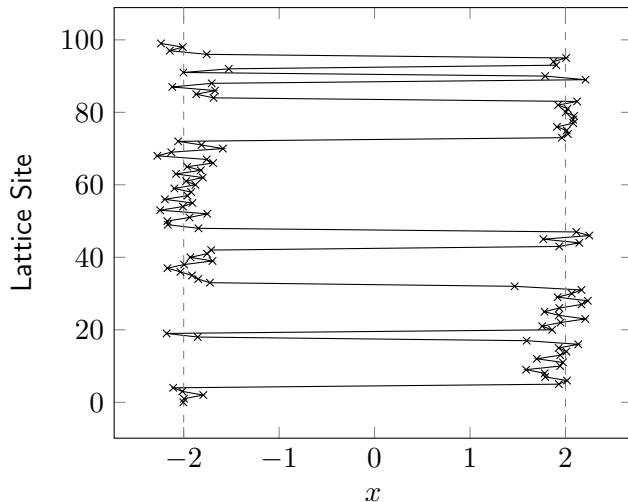
$$H_{HMC}(\mathbf{x}, \mathbf{p}) = \sum_{i=0}^{N-1} \frac{p_i^2}{2} + \sum_{i=0}^{N-1} a \left[\frac{1}{2} m \left(\frac{x_{i+1} - x_i}{a} \right)^2 + \lambda (x_i^2 - f^2)^2 \right]$$

Anharmonic Oscillator



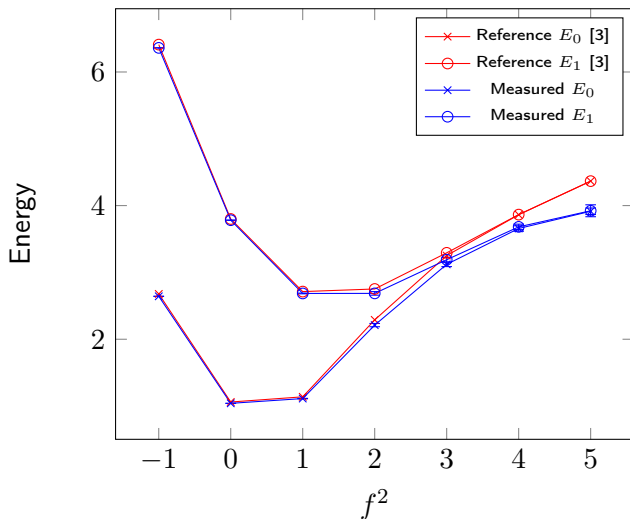
Anharmonic potential parameterisation, wells coincide with minima at $\pm f$ forming symmetric double wells.

Anharmonic Oscillator Typical Configuration



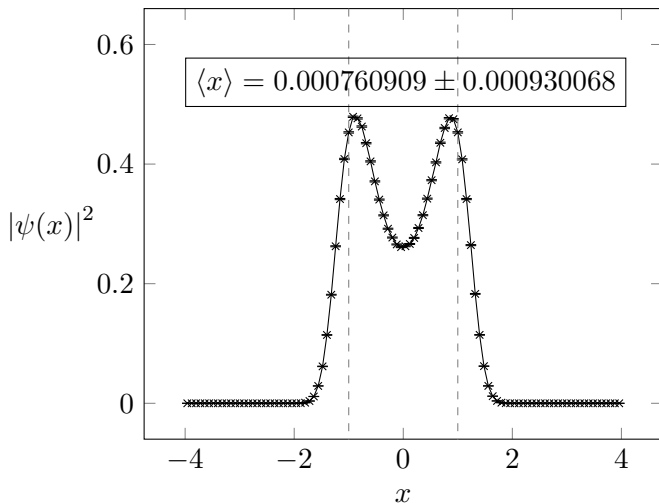
Typical equilibrium configuration on 100 site lattice at spacing $a = 1$ with anharmonic potential $\lambda = 1, f = 1$.

Anharmonic Oscillator Expectation Values



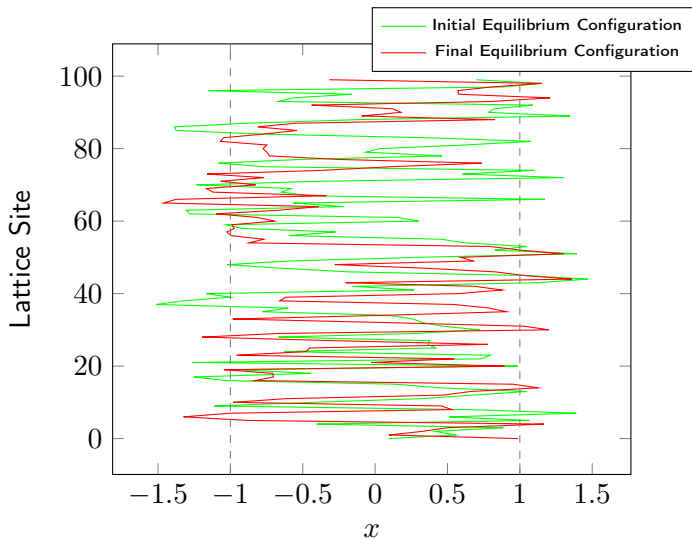
Ground and first excited state energy eigenvalues on 1000 site lattice at spacing $a = 0.1$ with anharmonic potential $\lambda = 1$ for a range of f values.

Anharmonic Oscillator Ground State Density Function



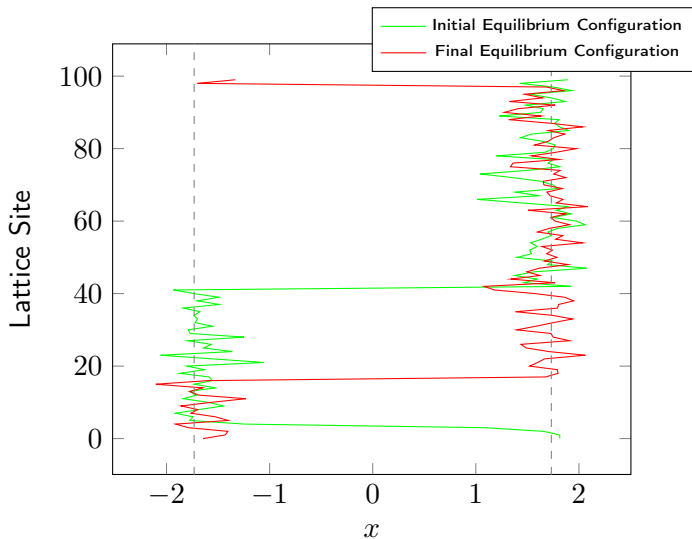
Ground state probability density function on 100 site lattice of spacing $a = 1$ with anharmonic potential $\lambda = 1, f = 1$.

Isolated Modes $\lambda = 1, f = 1$



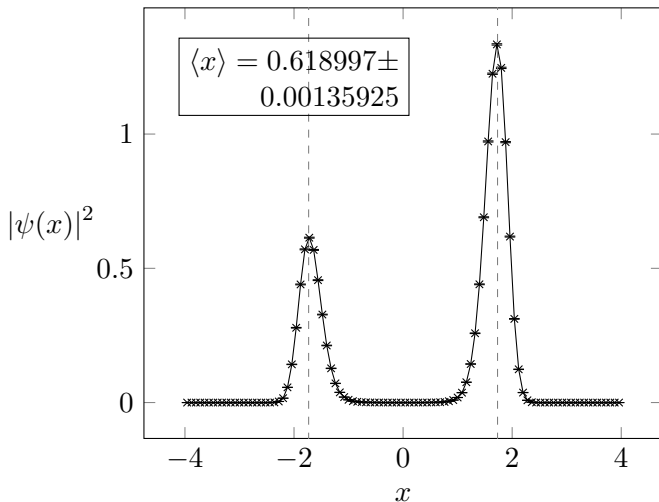
Initial and final equilibrium configurations after 100000 iterations on 100 site lattice at spacing $a = 1$.

Isolated Modes $\lambda = 1, f = \sqrt{3}$



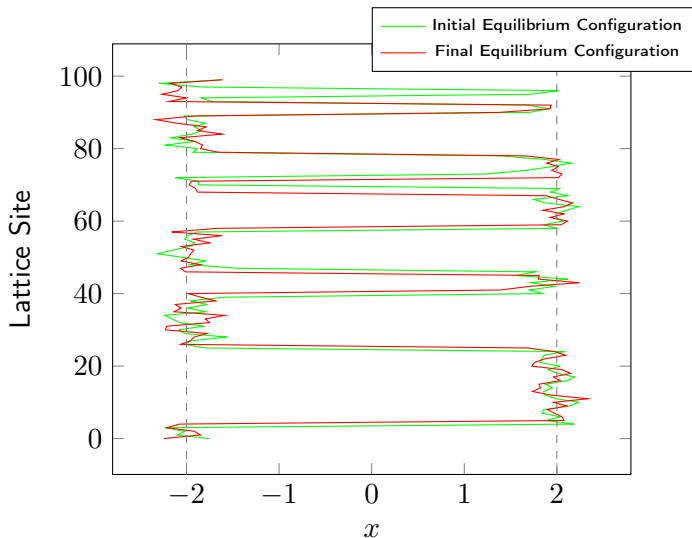
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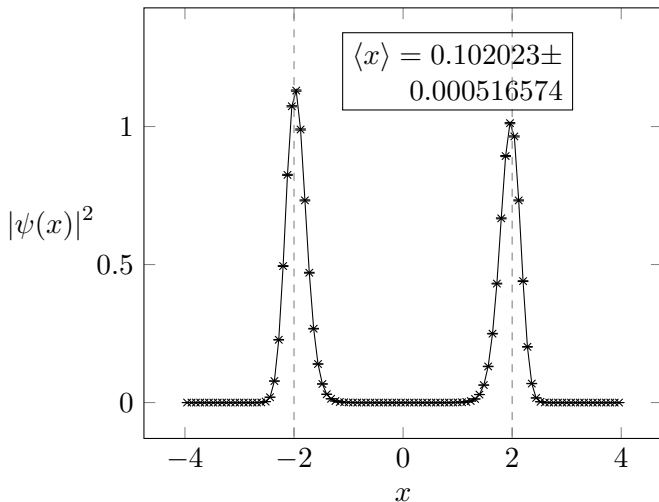
Asymmetric density function and non zero mean position.

Isolated Modes $\lambda = 1, f = 2$



Initial and final equilibrium configurations after 100000 iterations on 100 site lattice at spacing $a = 1$.

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Asymmetric density function and non zero mean position.

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 - ▶ Multiply (divide) momentum variables during the numerical integration of Hamilton's equations by a tempering parameter α in first (second) half of the trajectory [4].

Tempering

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

Leapfrog Integration

Hamiltonian

Form of Hamiltonian for our simulation:

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

Leapfrog Integration

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Leapfrog Equations

Half step in momentum then full step in position then half step in position to go from t to $t + \epsilon$:

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

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

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

Leapfrog Integration

Tempered Leapfrog Equations First Half Trajectory

Multiply momentum variables by $\sqrt{\alpha}$ before first half step in momentum and after second half step during first half of trajectory:

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

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

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

Leapfrog Integration

Tempered Leapfrog Equations Second Half Trajectory

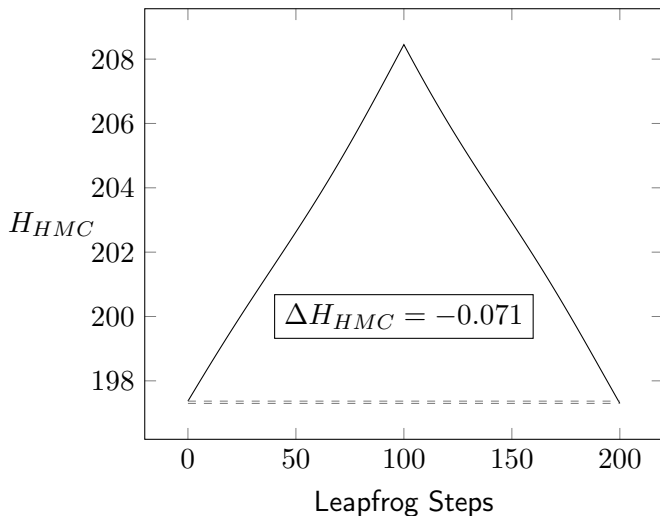
Divide momentum variables by $\sqrt{\alpha}$ before first half step in momentum and after second half step during second half of trajectory:

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

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

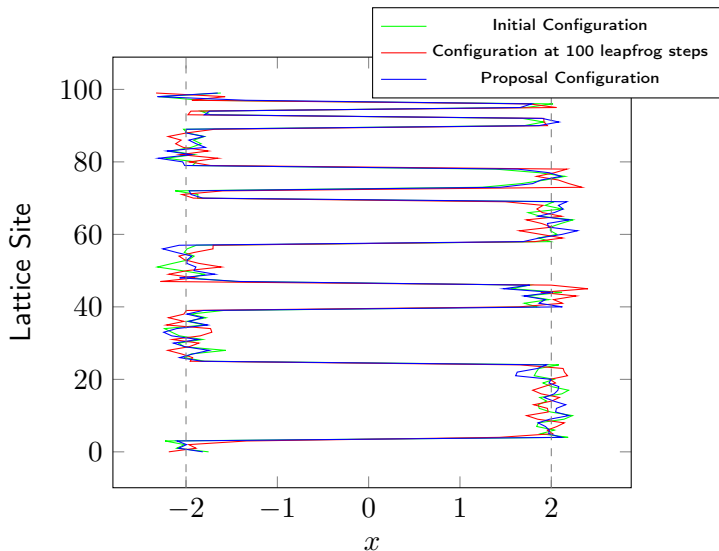
$$p_i(t + \epsilon) = \frac{1}{\sqrt{\alpha}} \left(p_i(t + \epsilon/2) - \epsilon/2 \frac{\partial U}{\partial q_i}(\mathbf{q}(t + \epsilon)) \right)$$

Molecular Dynamics Hamiltonian Evolution $\alpha = 1.001$



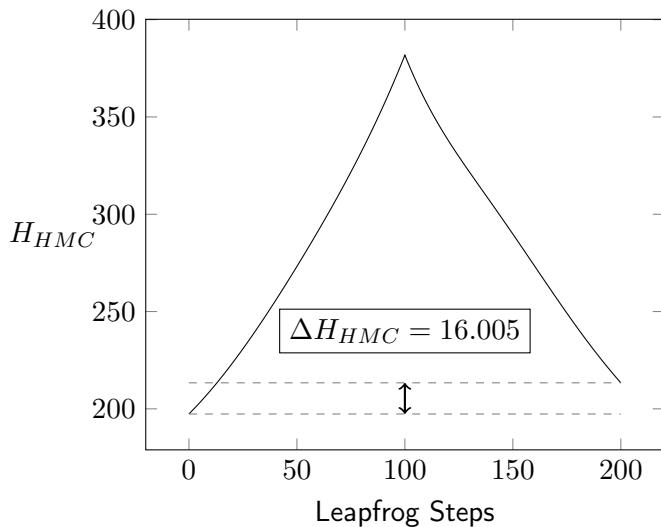
Evolution of HMC Hamiltonian along tempered leapfrog trajectory for 100 site lattice at spacing $a = 1$ with anharmonic potential $\lambda = 1, f = 2$.

Molecular Dynamics Configuration Evolution $\alpha = 1.001$



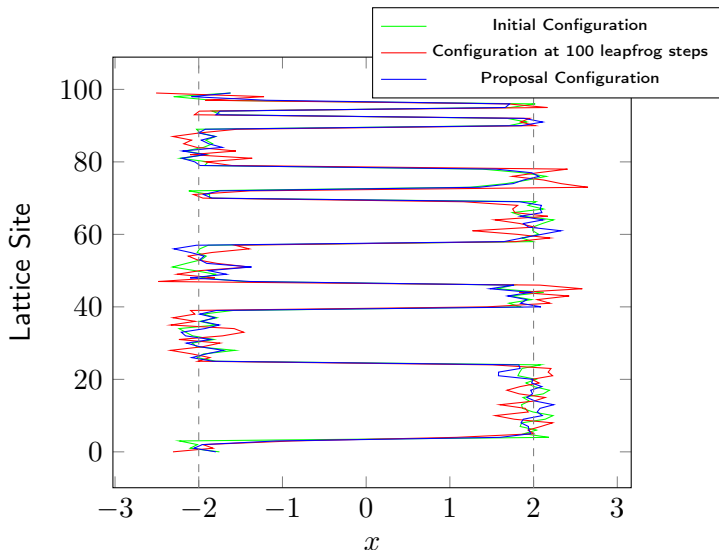
Evolution of the equilibrium configuration along the tempered leapfrog trajectory.

Molecular Dynamics Hamiltonian Evolution $\alpha = 1.01$



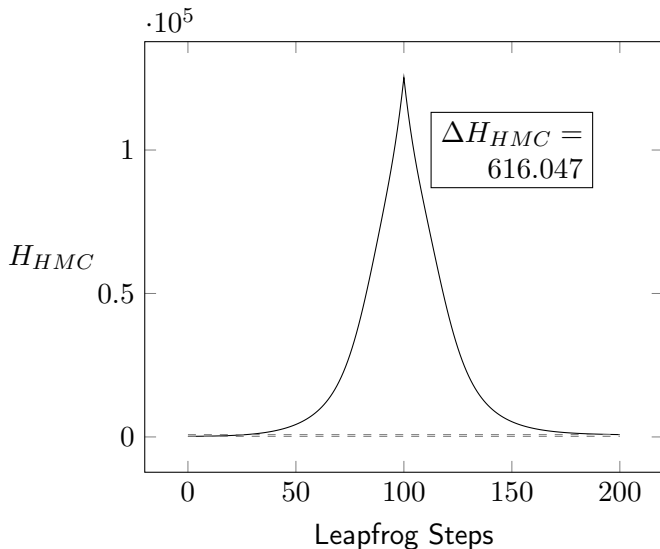
Evolution of HMC Hamiltonian along tempered leapfrog trajectory.

Molecular Dynamics Configuration Evolution $\alpha = 1.01$



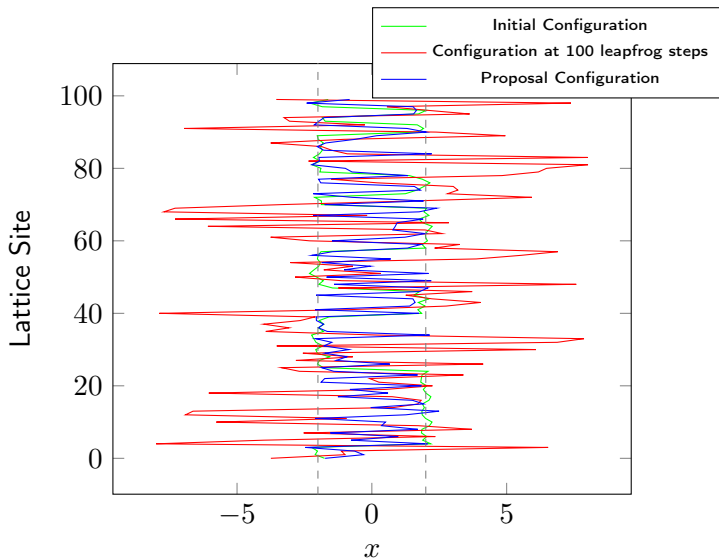
Evolution of the equilibrium configuration along the tempered leapfrog trajectory.

Molecular Dynamics Hamiltonian Evolution $\alpha = 1.05$



Evolution of HMC Hamiltonian along tempered leapfrog trajectory.

Molecular Dynamics Configuration Evolution $\alpha = 1.05$



Evolution of the equilibrium configuration along the tempered leapfrog trajectory.

Conclusion

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

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Conclusion

- ▶ Did it work?
 - ▶ Successfully reproduced theoretical 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 - *local tempering*.

References I



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Volume Preservation on Phase Space I

Can define the mappings on phase space:

$$\mathcal{T}_q(\epsilon) \begin{pmatrix} \mathbf{q} \\ \mathbf{p} \end{pmatrix} = \begin{pmatrix} \mathbf{q} + \epsilon \underline{\nabla}_{\mathbf{p}} K(\mathbf{p}) \\ \mathbf{p} \end{pmatrix},$$

$$\mathcal{T}_p(\epsilon) \begin{pmatrix} \mathbf{q} \\ \mathbf{p} \end{pmatrix} = \begin{pmatrix} \mathbf{q} \\ \mathbf{p} - \epsilon \underline{\nabla}_{\mathbf{q}} U(\mathbf{q}) \end{pmatrix},$$

with a slight abuse of notation the Jacobians of these mappings will be of the form:

$$J = \det \begin{pmatrix} \frac{\partial q'_i}{\partial q_j} & \frac{\partial q'_i}{\partial p_j} \\ \frac{\partial p'_i}{\partial q_j} & \frac{\partial p'_i}{\partial p_j} \end{pmatrix}$$

Volume Preservation on Phase Space II

so that:

$$J_q = \det \begin{pmatrix} \delta_{ij} & \epsilon \partial_{p_i} \partial_{p_j} K(\mathbf{p}) \\ 0 & \delta_{ij} \end{pmatrix} = 1$$
$$J_p = \det \begin{pmatrix} \delta_{ij} & 0 \\ -\epsilon \partial_{q_i} \partial_{q_j} U(\mathbf{q}) & \delta_{ij} \end{pmatrix} = 1.$$

Single leapfrog step of size epsilon can be written as:

$$\mathcal{T}(\epsilon) = \mathcal{T}_p(\epsilon/2) \circ \mathcal{T}_q(\epsilon) \circ \mathcal{T}_p(\epsilon/2).$$

We may write the mapping that via leapfrog integration takes us from the start to the end of the trajectory as:

$$\text{traj}(\epsilon, l) = (\mathcal{T}(\epsilon))^l,$$

which has Jacobian 1, therefore volume preserved.

Volume Preservation on Phase Space with Tempering I

Can define the mappings on phase space:

$$\mathcal{T}_{p_1}(\epsilon, \alpha) \begin{pmatrix} \mathbf{q} \\ \mathbf{p} \end{pmatrix} = \begin{pmatrix} \mathbf{q} \\ \sqrt{\alpha} \mathbf{p} - \epsilon \underline{\nabla}_{\mathbf{q}} U(\mathbf{q}) \end{pmatrix},$$

$$\mathcal{T}_q(\epsilon) \begin{pmatrix} \mathbf{q} \\ \mathbf{p} \end{pmatrix} = \begin{pmatrix} \mathbf{q} + \epsilon \underline{\nabla}_{\mathbf{p}} K(\mathbf{p}) \\ \mathbf{p} \end{pmatrix},$$

$$\mathcal{T}_{p_2}(\epsilon, \alpha) \begin{pmatrix} \mathbf{q} \\ \mathbf{p} \end{pmatrix} = \begin{pmatrix} \mathbf{q} \\ \sqrt{\alpha} (\mathbf{p} - \epsilon \underline{\nabla}_{\mathbf{q}} U(\mathbf{q})) \end{pmatrix},$$

Volume Preservation on Phase Space with Tempering II

Jacobians of these mappings:

$$J_{p_1} = \det \begin{pmatrix} \delta_{ij} & 0 \\ -\epsilon \partial q_i \partial q_j U(\mathbf{q}) & \sqrt{\alpha} \delta_{ij} \end{pmatrix} = \alpha^{\frac{d}{2}}$$

$$J_q = \det \begin{pmatrix} \delta_{ij} & \epsilon \partial p_i \partial p_j K(\mathbf{p}) \\ 0 & \delta_{ij} \end{pmatrix} = 1$$

$$J_{p_2} = \det \begin{pmatrix} \delta_{ij} & 0 \\ -\sqrt{\alpha} \epsilon \partial q_i \partial q_j U(\mathbf{q}) & \sqrt{\alpha} \delta_{ij} \end{pmatrix} = \alpha^{\frac{d}{2}}.$$

Leapfrog step in the first half of the trajectory:

$\mathcal{T}(\alpha, \epsilon) = \mathcal{T}_{p_2}(\alpha, \epsilon/2) \circ \mathcal{T}_q(\epsilon) \circ \mathcal{T}_{p_1}(\alpha, \epsilon/2)$, with Jacobian α^d ,

second half trajectory as

$\mathcal{T}(1/\alpha, \epsilon) = \mathcal{T}_{p_2}(1/\alpha, \epsilon/2) \circ \mathcal{T}_q(\epsilon) \circ \mathcal{T}_{p_1}(1/\alpha, \epsilon/2)$ with Jacobian $1/\alpha^d$.

Volume Preservation on Phase Space with Tempering III

The mapping which via the leapfrog equations takes us from the start to the end of the trajectory can be written as:

$$\text{traj}(\alpha, \epsilon, l) = [\mathcal{T}(1/\alpha, \epsilon)]^{\frac{l}{2}} \circ [\mathcal{T}(\alpha, \epsilon)]^{\frac{l}{2}}$$

which has Jacobian $J_{\text{traj}} = [\alpha^d]^{\frac{l}{2}} [1/\alpha^d]^{\frac{l}{2}} = 1$, therefore volume preserved.

Ground State Expectation Values I

$$\langle \hat{A} \rangle = \frac{\text{Tr} \left(e^{-(\tau_b - \tau_a) \hat{H} / \hbar} \hat{A} \right)}{\text{Tr} \left(e^{-(\tau_b - \tau_a) \hat{H} / \hbar} \right)}$$

Following the discretisation theory as for the transition amplitude[5]:

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

Limit that $\tau_b - \tau_a \rightarrow \infty$ for a large enough lattice:

$$\begin{aligned} \langle \hat{A} \rangle &= \frac{\sum_{n=0}^{\infty} e^{-\frac{1}{\hbar} E_n (\tau_b - \tau_a)} \langle n | \hat{A} | n \rangle}{\sum_{n=0}^{\infty} e^{-\frac{1}{\hbar} E_n (\tau_b - \tau_a)}} \\ &= \langle 0 | \hat{A} | 0 \rangle. \end{aligned}$$

Quantum Virial Theorem I

$$2 \langle n | \hat{T} | n \rangle = \langle n | \hat{x} \hat{V}'(\hat{x}) | n \rangle$$

giving:

$$E_0 = \left\langle \frac{1}{2} x V'(x) + V(x) \right\rangle$$

so for harmonic oscillator:

$$E_0 = \mu^2 \langle x^2 \rangle,$$

and anharmonic oscillator:

$$E_0 = 3\lambda \langle x^4 \rangle - 4\lambda f^2 \langle x^2 \rangle + \lambda f^4.$$