Accelerated Tempering Dynamics in HMC Simulations of Lattice Field Theory

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  - Calculating properties of Quantum Mechanical Systems.

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- 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

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

Probability density of $(x_b, t_b) \to (x_a, t_a)$.
Integral over all paths between (x_b, t_b) and (x_a, t_a).

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Minkowski Action

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

The Path Integral

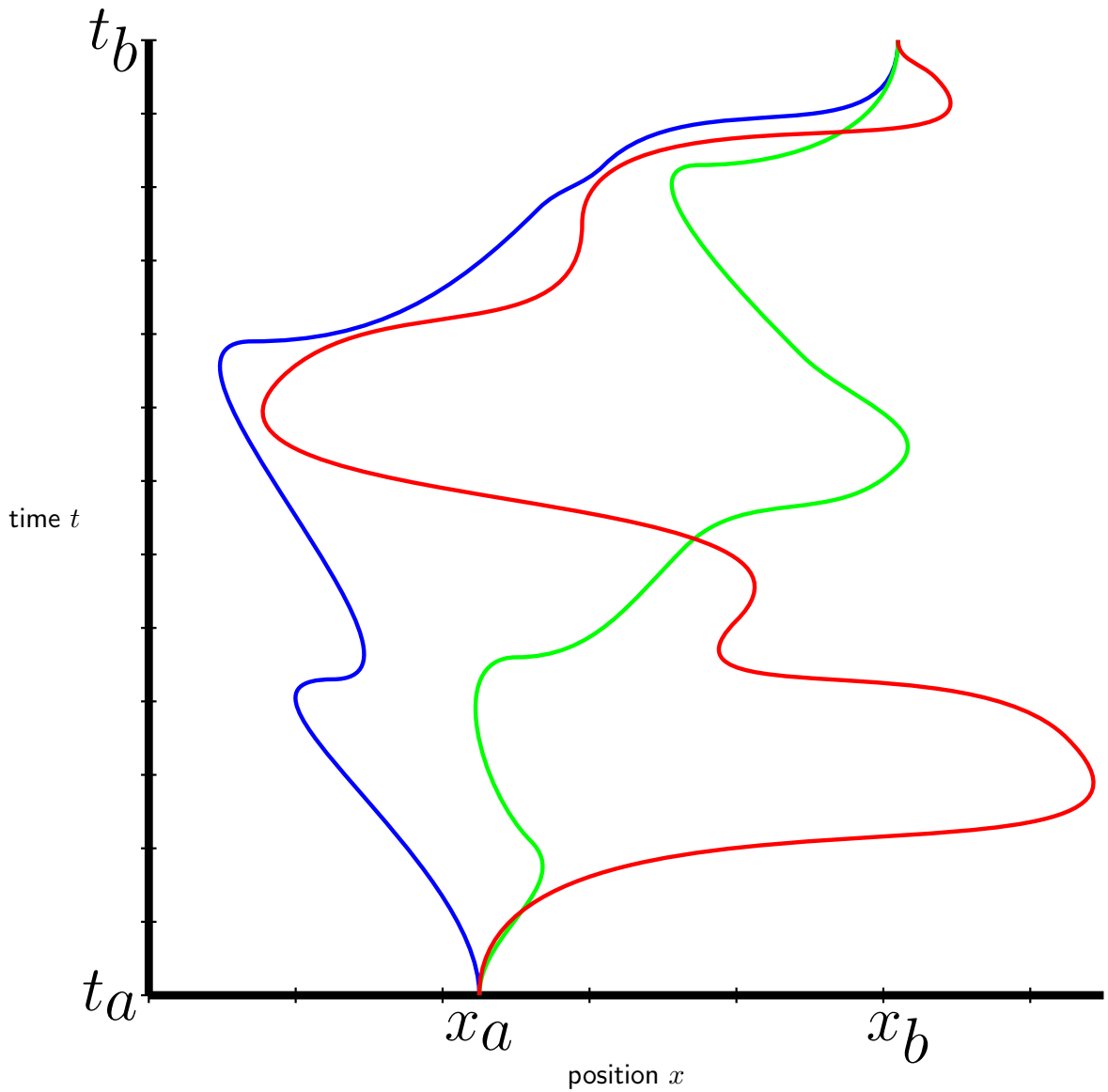

Figure 1: Three possible paths from (x_a, t_a) to (x_b, t_b).

Discrete Time Lattice

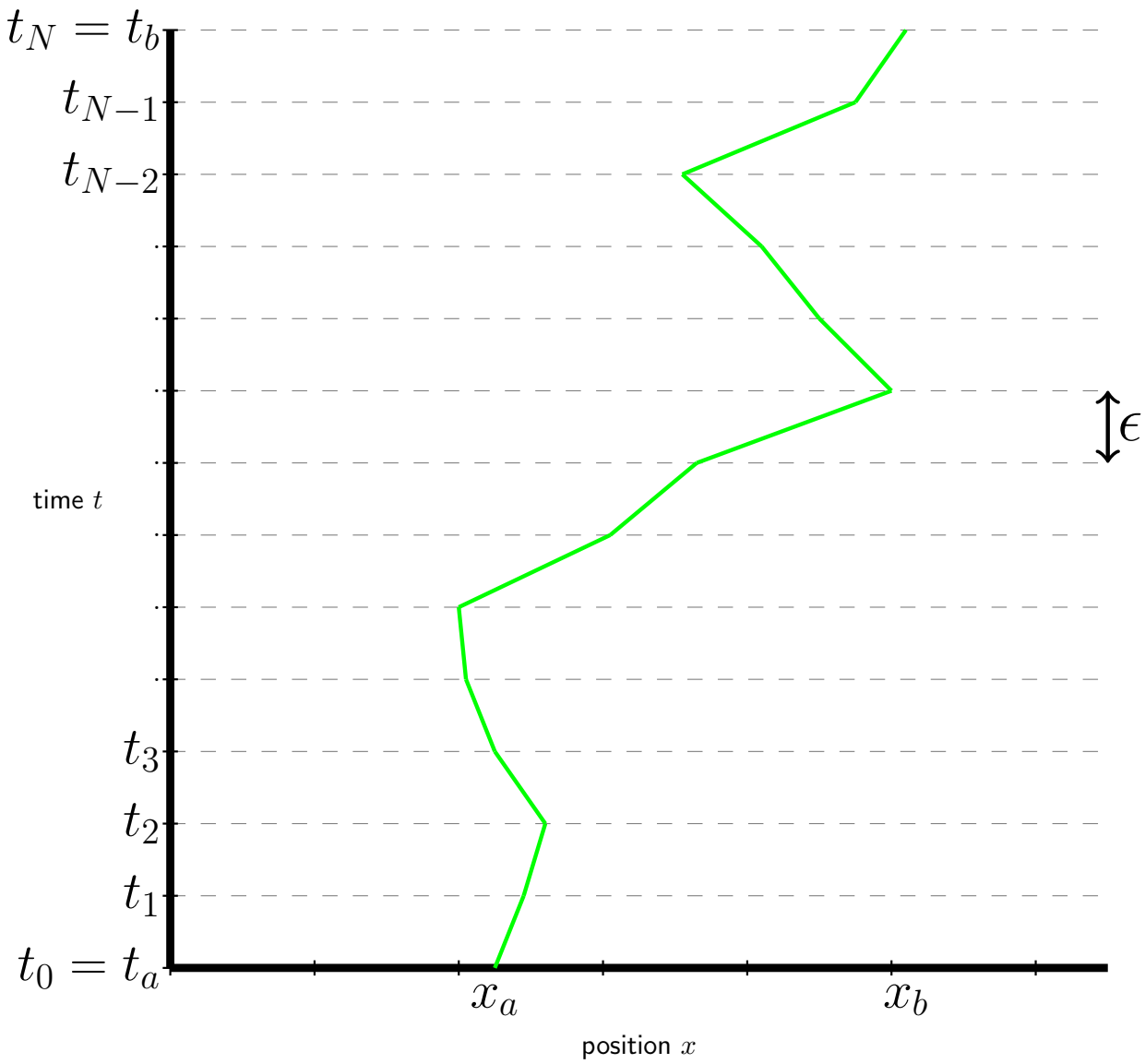

Figure 2: Discretising time and a path from (x_a, t_a) to (x_b, t_b) onto a lattice of time spacing ϵ.

Discrete Time Lattice

Configuration

Specific path through lattice, each lattice variable specified:

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

$$x_i = x\left(t_i\right)$$

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Substitution for imaginary time:

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Wick Rotation

Substitution for imaginary time:

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

$$a = i\epsilon$$

Connecting to Statistical Mechanics

Discrete Euclidean Path Integral

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

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

Connecting to Statistical Mechanics

Quantum Expectation Values

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

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

Monte Carlo

Expectation Value

Integrals cannot be computed analytically:

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

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Monte Carlo Estimate

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

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

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Boltzmann Distribution

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

Introduce fictitious momentum variable to go with each lattice variable:

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

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HMC Hamiltonian

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

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

The Hybrid Monte Carlo Algorithm

HMC Algorithm

0. Provide initial configuration x.

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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).

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4. Return to step 1.

Harmonic Oscillator

The potential

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

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

Harmonic Oscillator Typical Configuration

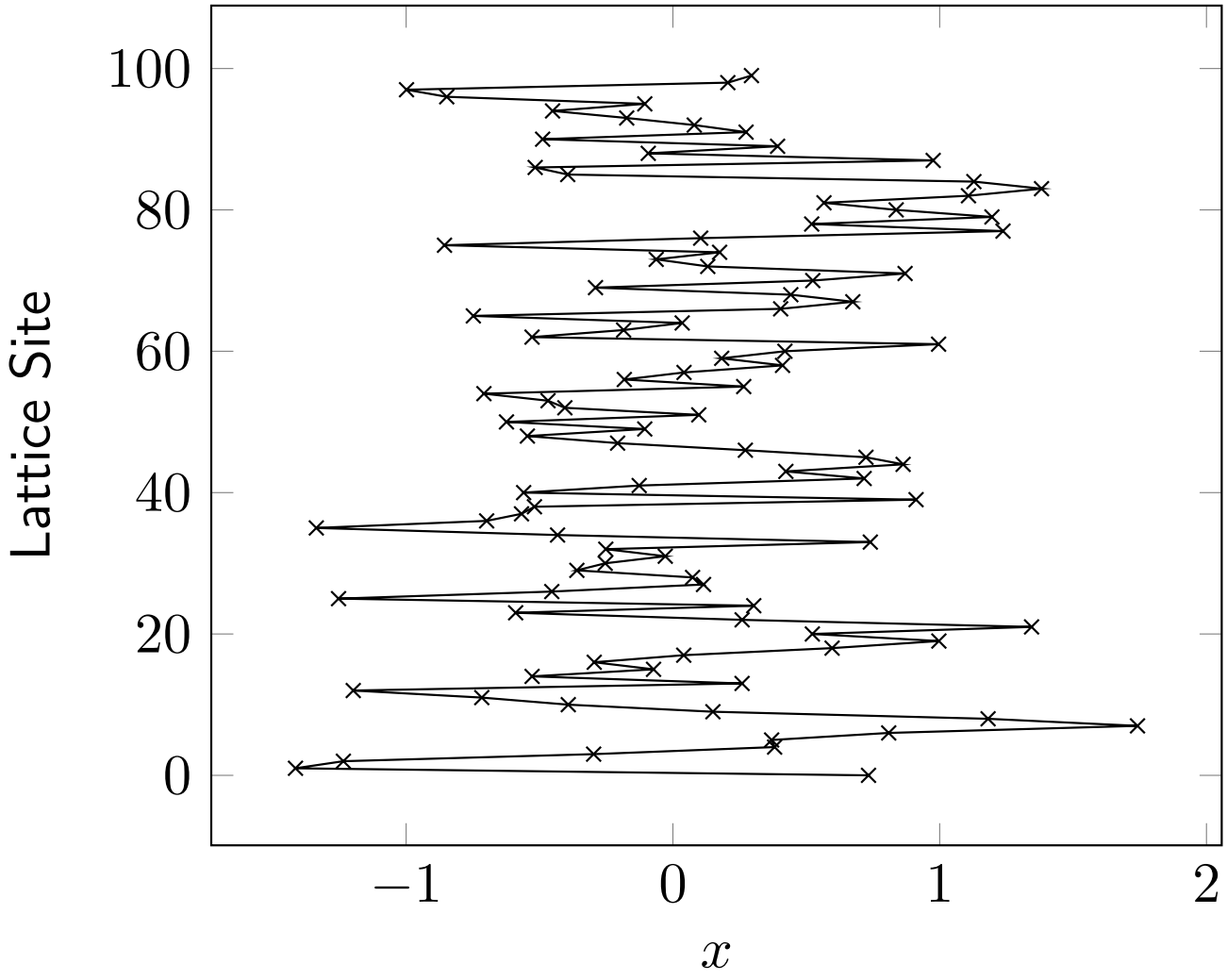

Figure 2: Typical equilibrium configuration on 100 site lattice at spacing $a = 1$ with harmonic potential $\mu = 1$.

Harmonic Oscillator Expectation Values

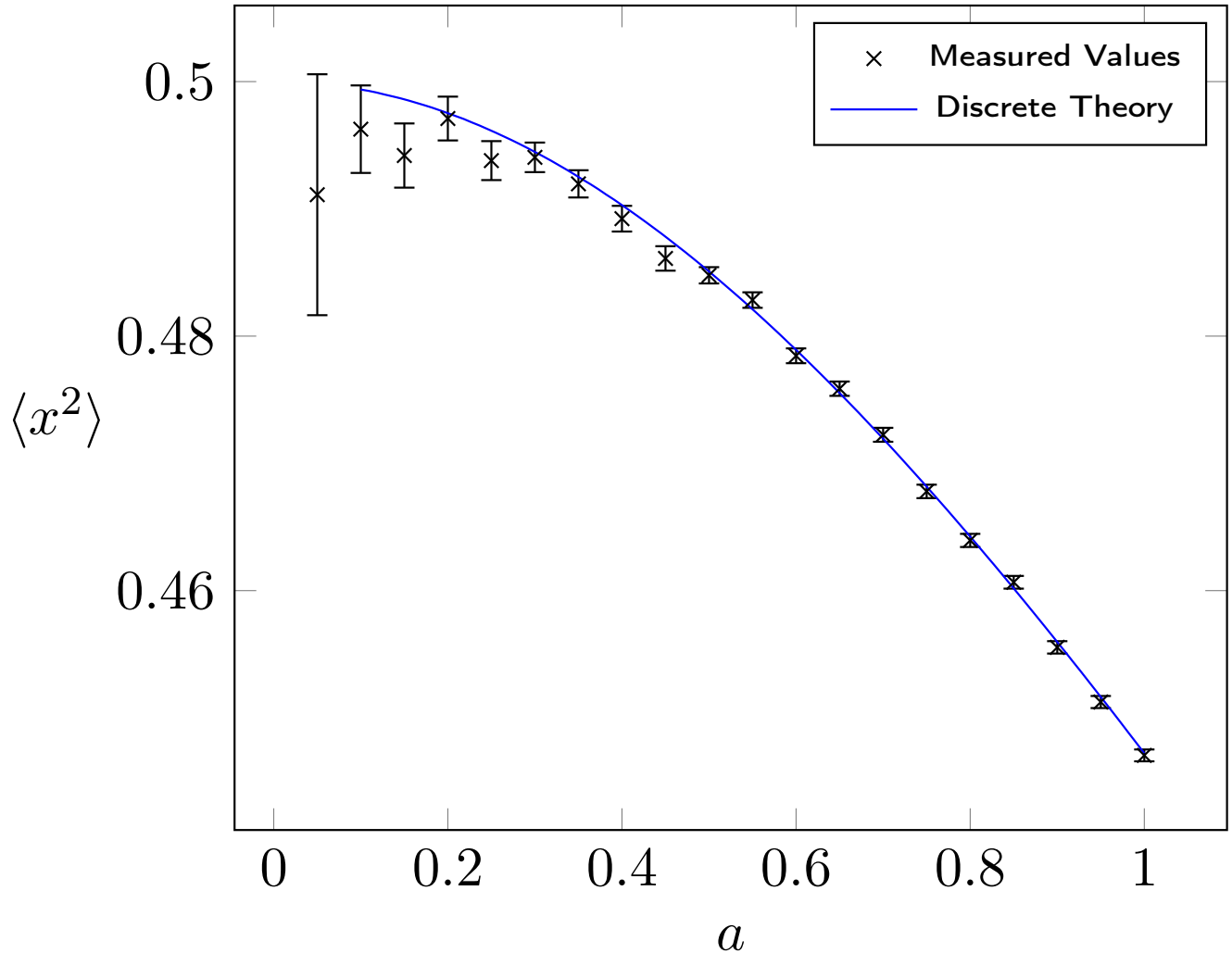

Figure 3: Mean position squared for a range of finite lattice spacings on a 100 site lattice with harmonic potential $\mu = 1$.

Harmonic Oscillator Ground State Probability Density

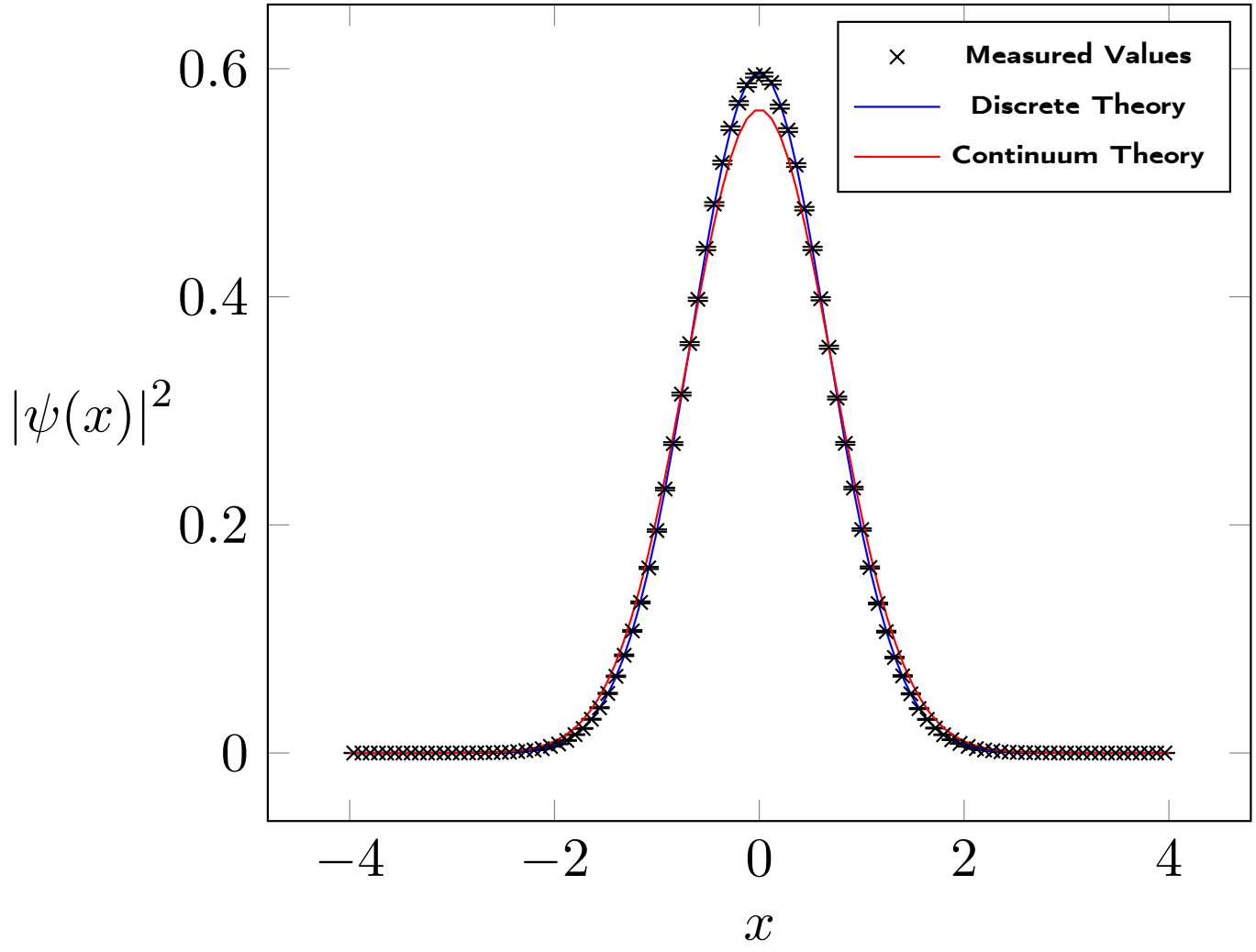

Figure 4: Ground state probability density function for 100 site lattice at spacing $a = 1$ for harmonic potential $\mu = 1$.

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Anharmonic Oscillator

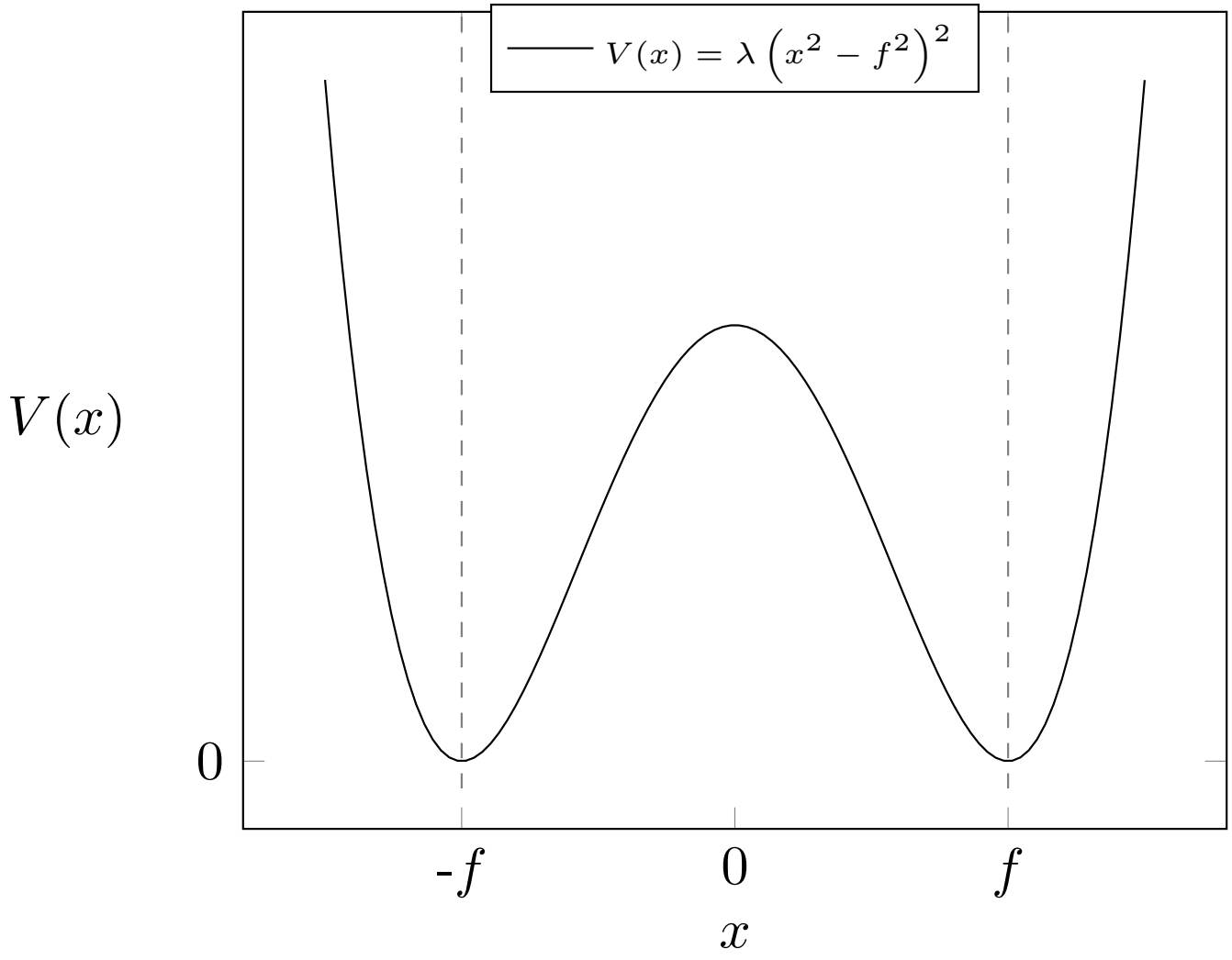

Figure 5: Anharmonic potential parameterisation, wells coincide with minima at $\pm f$ forming symmetric double wells.

Anharmonic Oscillator Typical Configuration

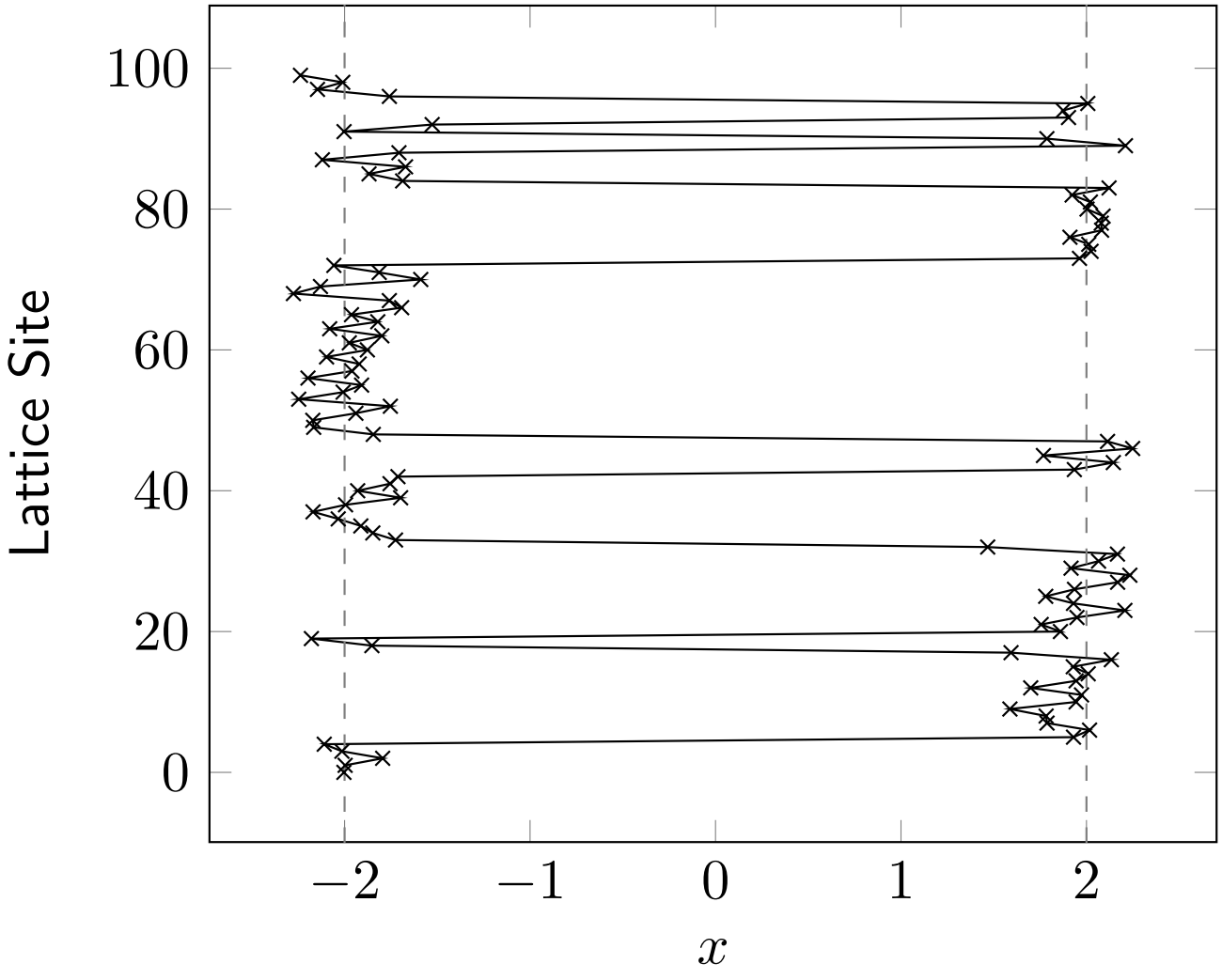

Figure 6: Typical equilibrium configuration on 100 site lattice at spacing $a = 1$ with anharmonic potential $\lambda = 1, f = 1$.

Anharmonic Oscillator Expectation Values

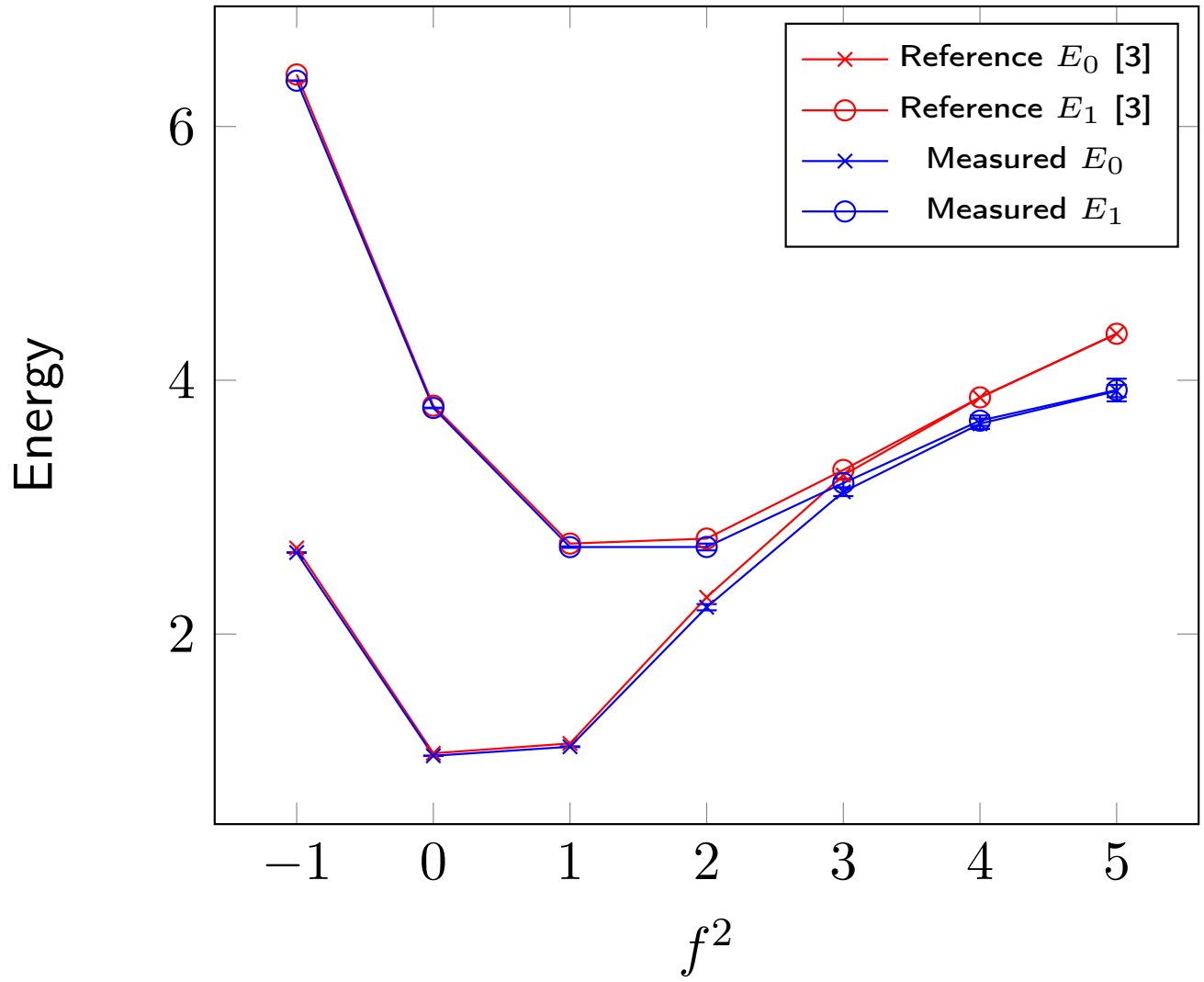

Figure 7: Ground and first excited state energy eigenvalues on 1000 site lattice at spacing $a = 0.1$ with anharmonic potential $\lambda = 1$ for a range of f values.

Anharmonic Oscillator Ground State Density Function

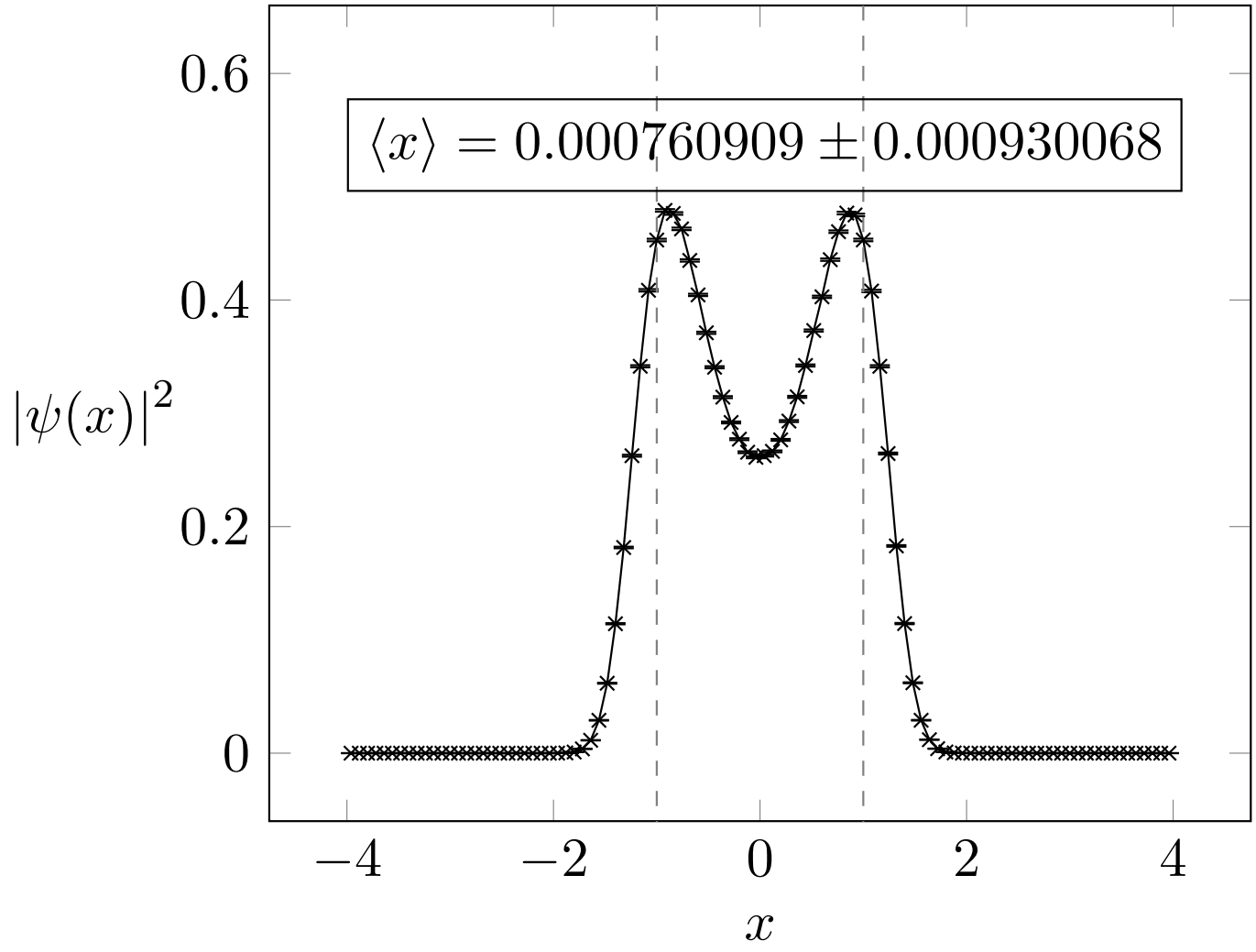

Figure 8: Ground state probability density function on 100 site lattice of spacing $a = 1$ with anharmonic potential $\lambda = 1, f = 1$.

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

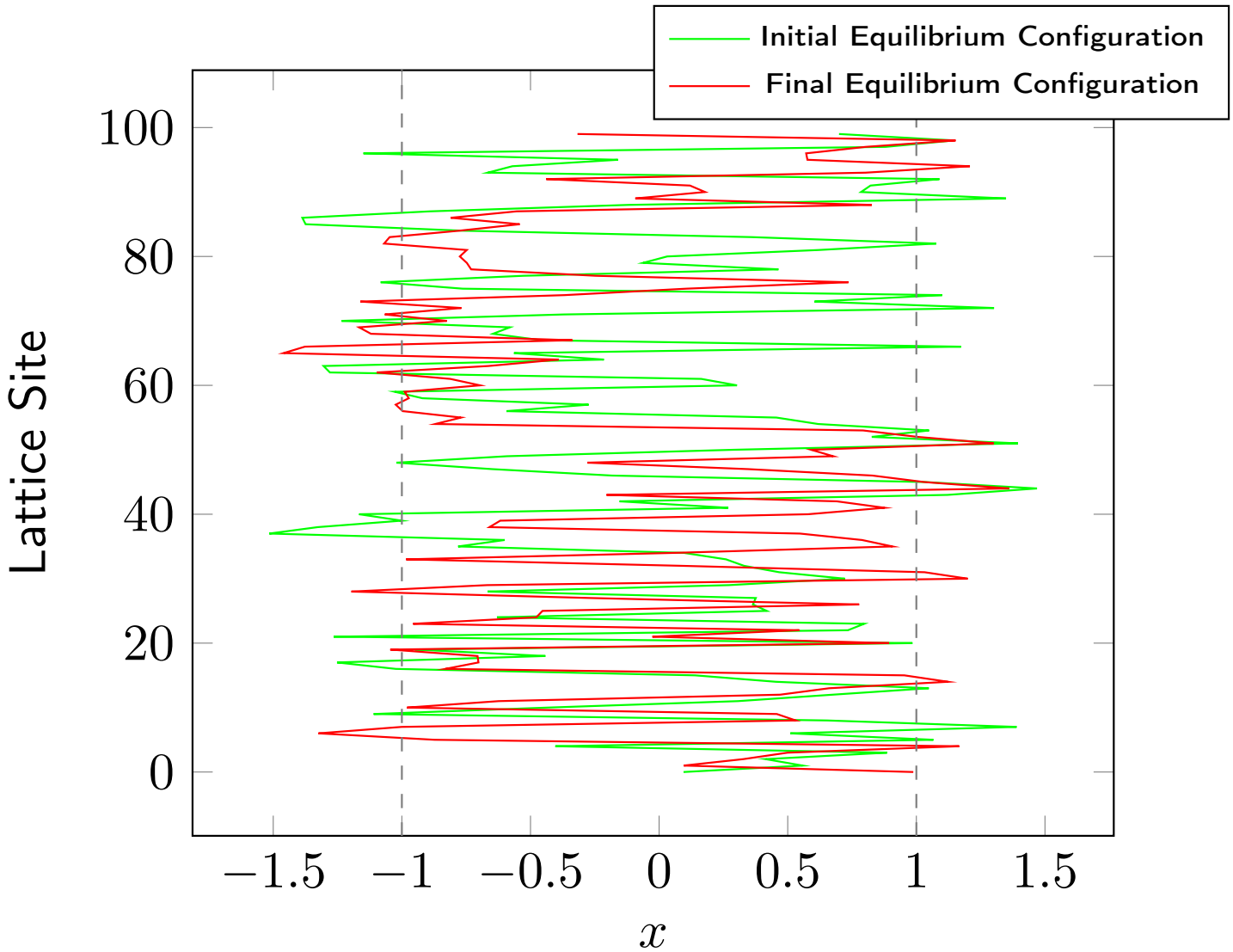

Figure 9: Initial and final equilibrium configurations after 100000 iterations on 100 site lattice at spacing $a = 1$.

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

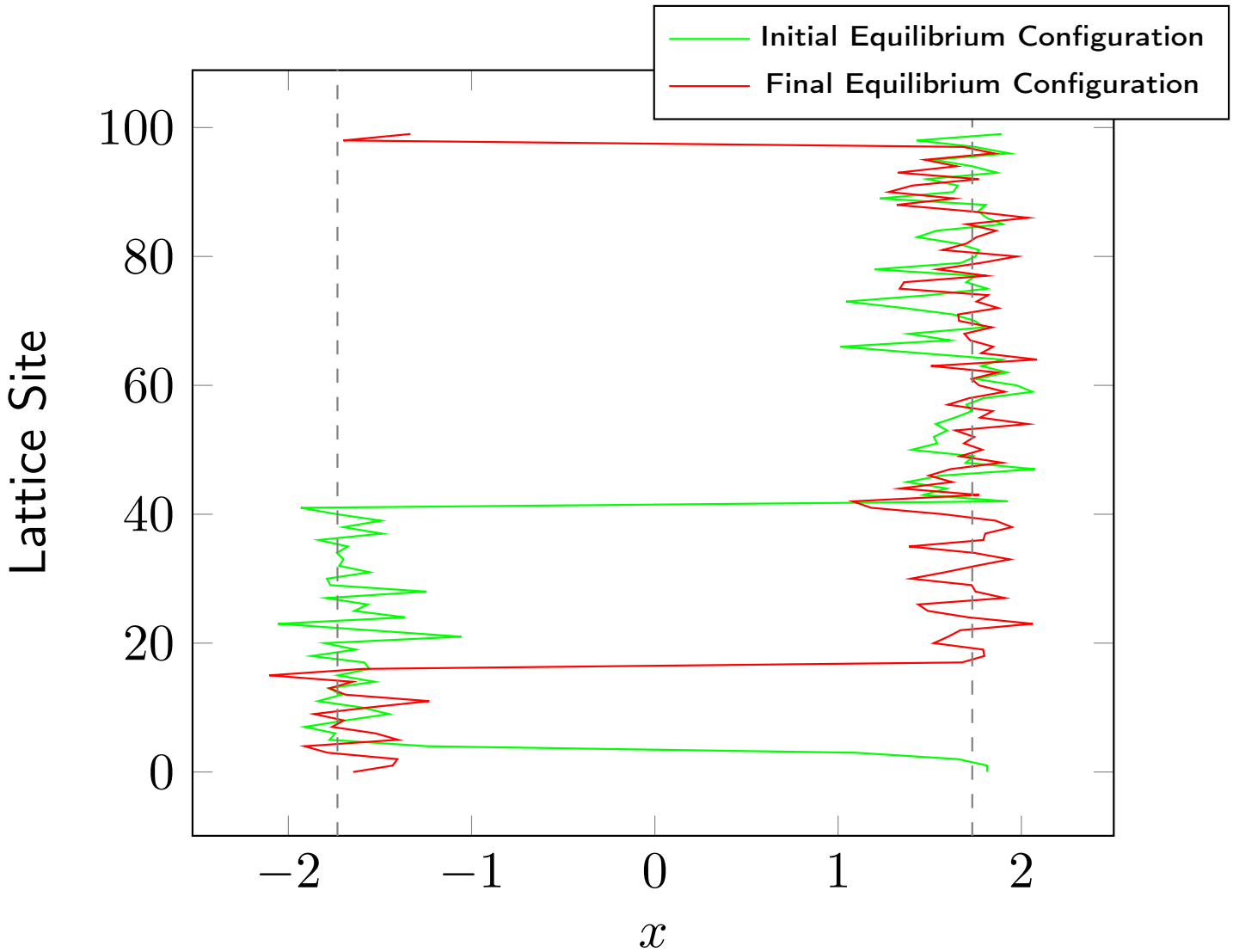

Figure 10: Initial and final equilibrium configurations after 100000 iterations on 100 site lattice at spacing $a = 1$.

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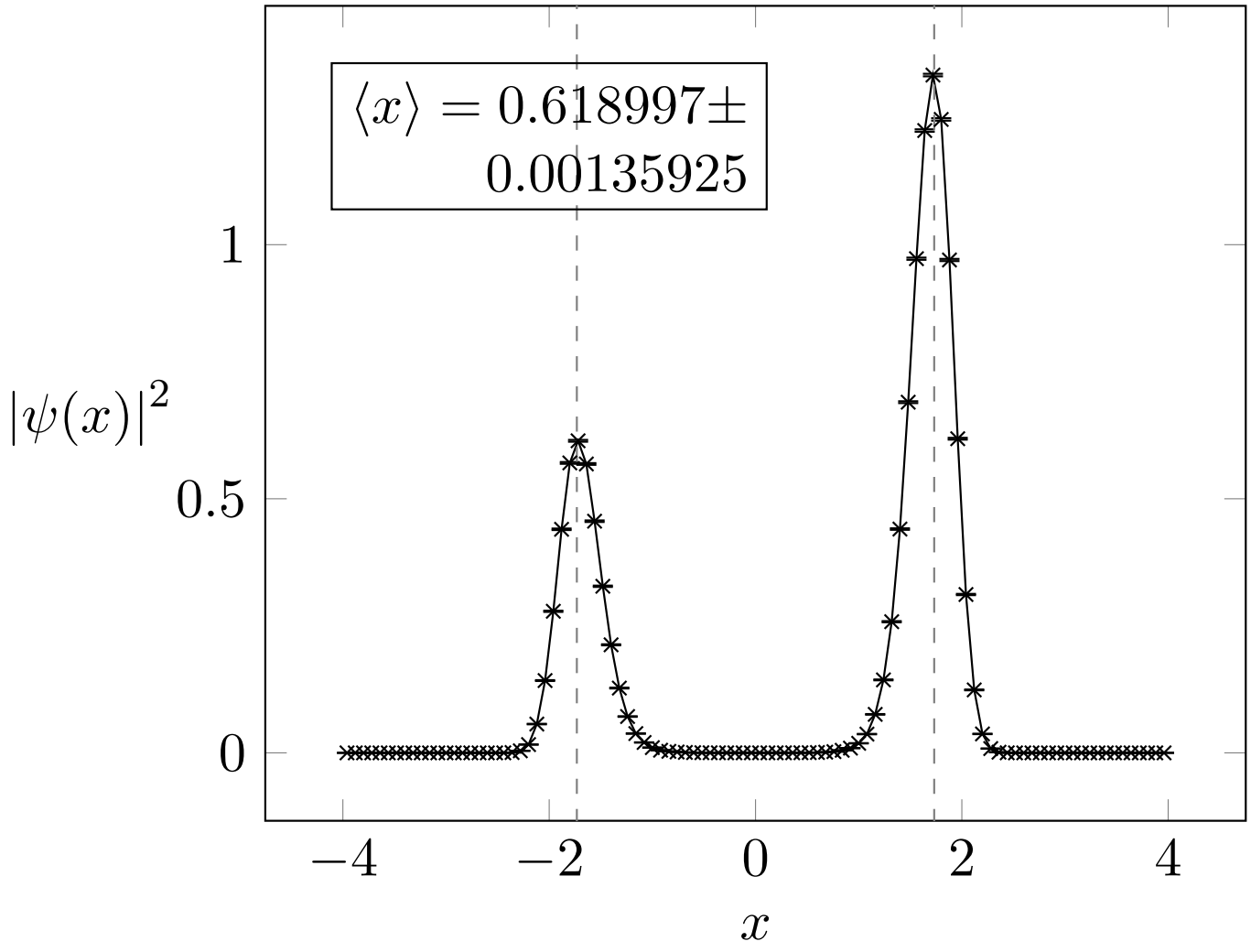


Figure 11: Asymmetric density function and non zero mean position.

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

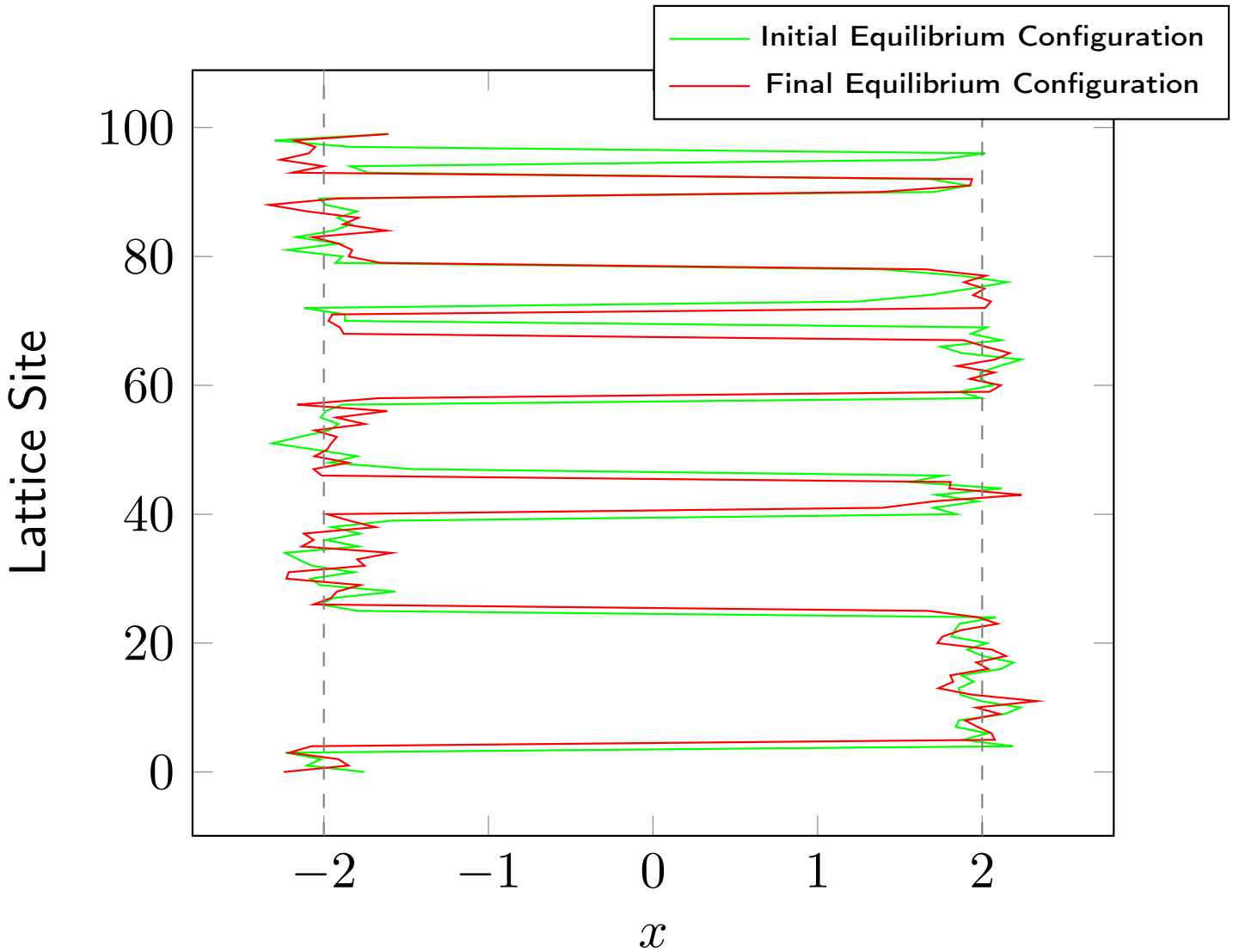
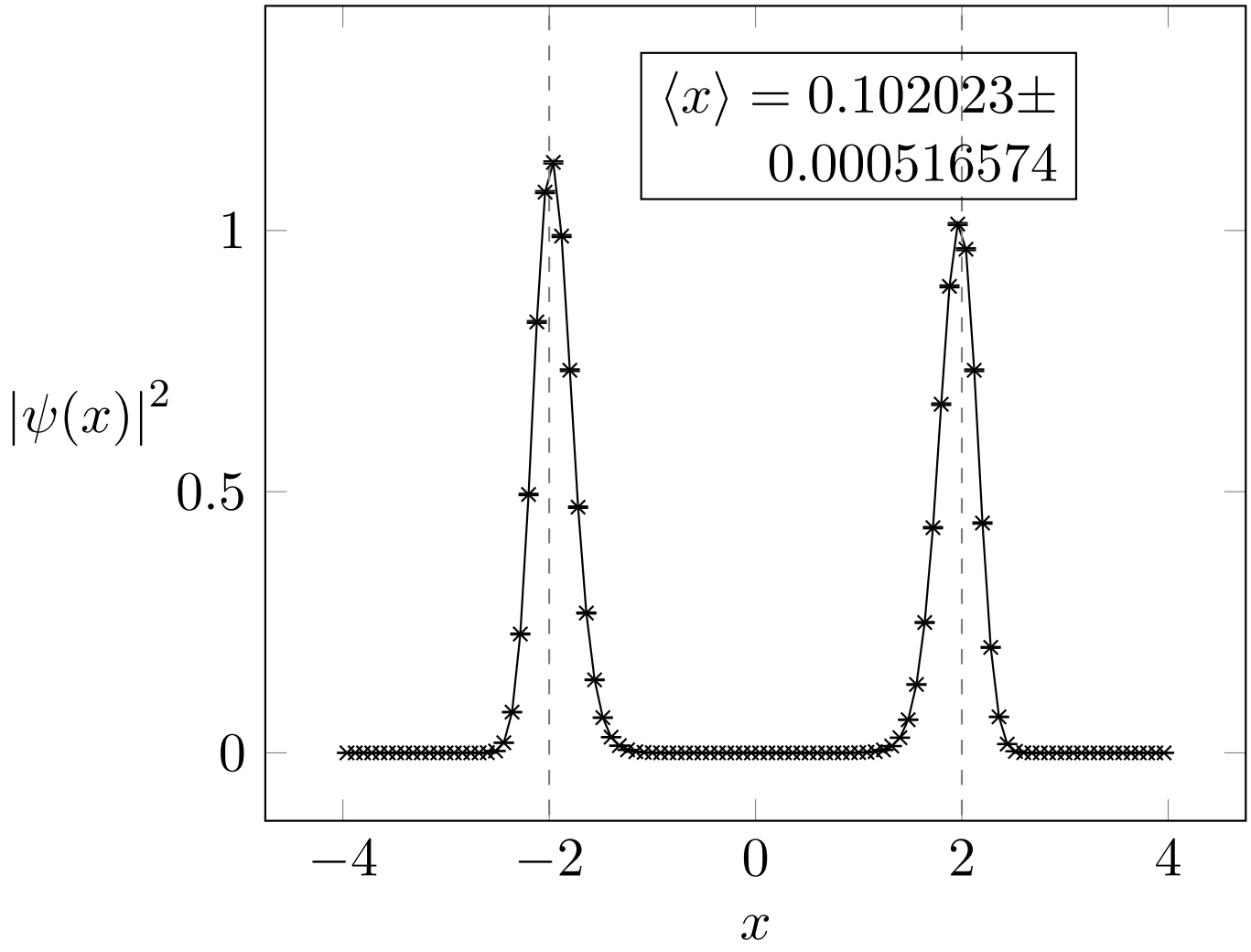


Figure 12: Initial and final equilibrium configurations after 100000 iterations on 100 site lattice at spacing $a = 1$.

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



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  - Method to sample from more diffuse probability distribution.

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- 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:

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

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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 $t + \epsilon$:

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

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

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

Leapfrog Integration

Tempered Leapfrog Equations First Half Trajectory

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

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

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

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

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

Molecular Dynamics Hamiltonian Evolution $\alpha = 1.001$

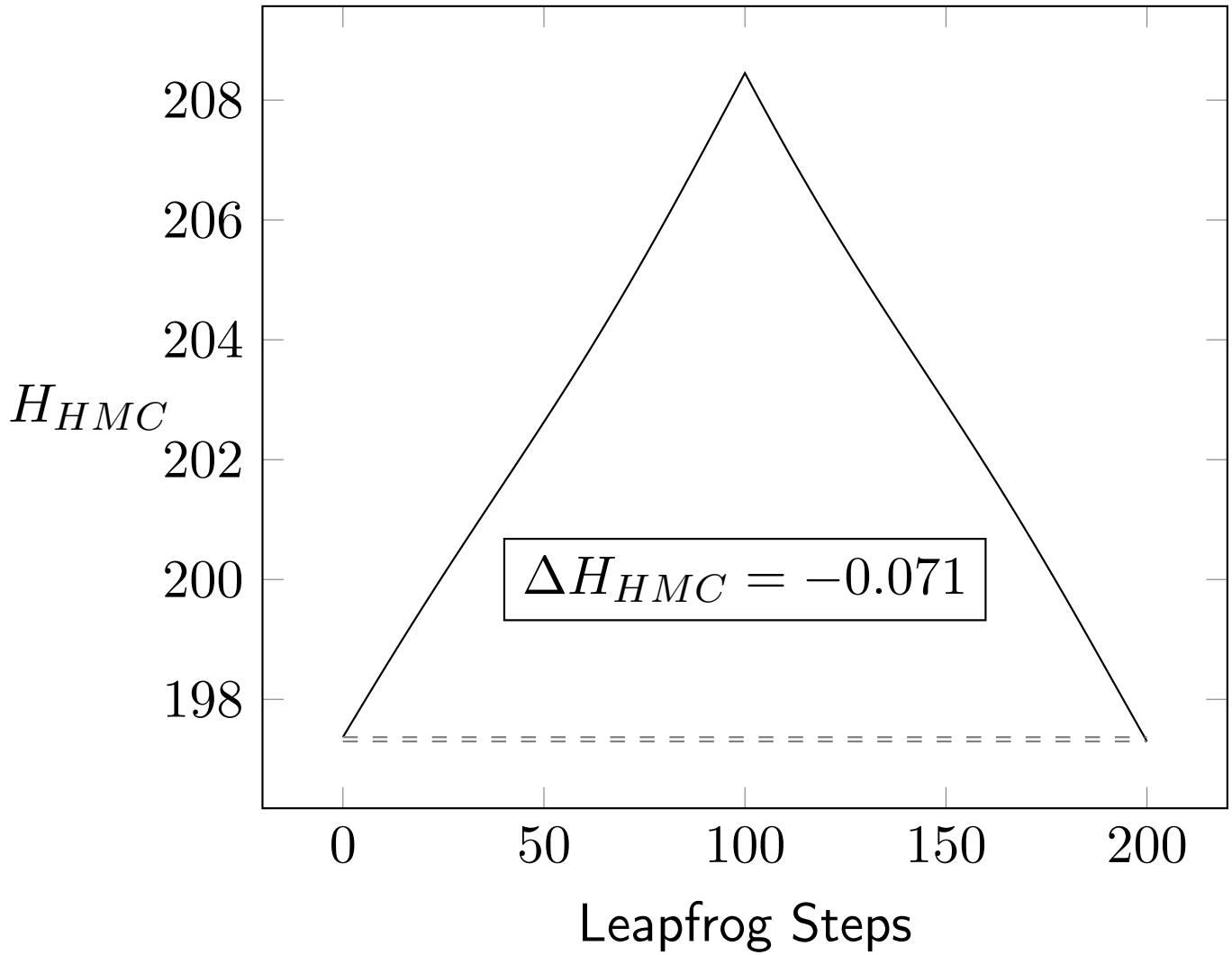

Figure 14: Evolution of HMC Hamiltonian along tempered leapfrog trajectory for 100 site lattice at spacing $a = 1$ with anharmonic potential $\lambda = 1, f = 2$.

Molecular Dynamics Configuration Evolution $\alpha = 1.001$

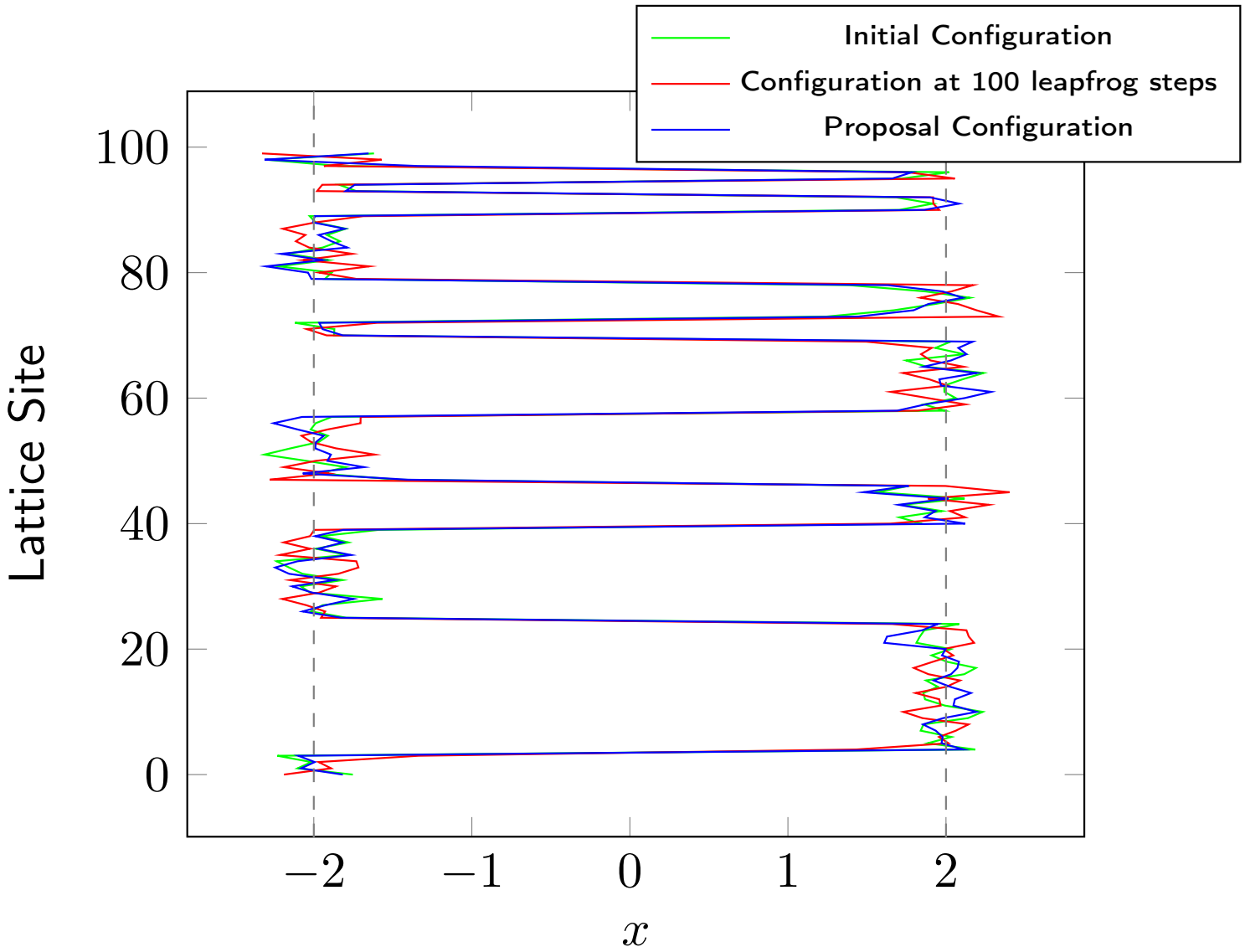

Figure 15: Evolution of the equilibrium configuration along the tempered leapfrog trajectory.

Molecular Dynamics Hamiltonian Evolution $\alpha = 1.01$

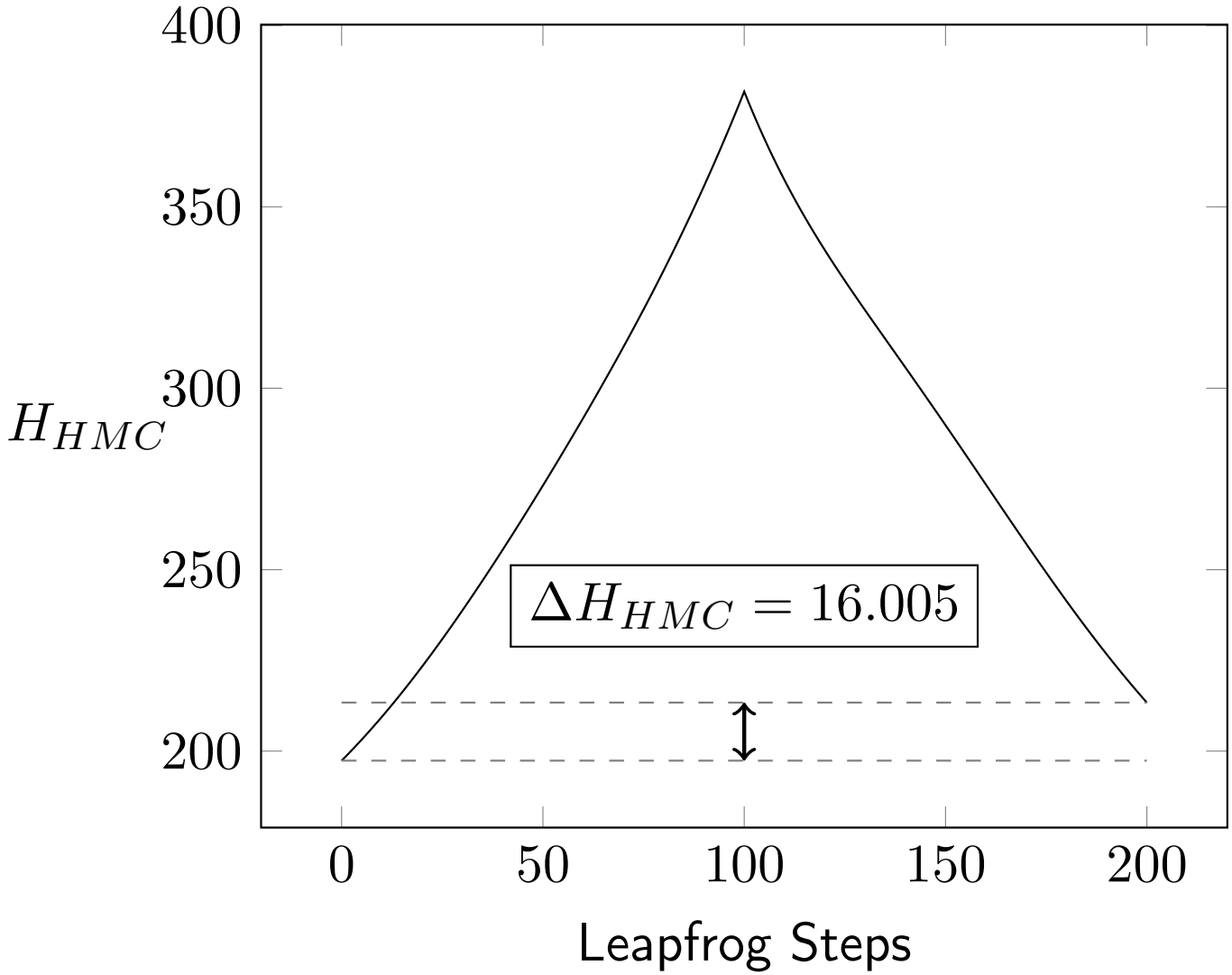

Figure 16: Evolution of HMC Hamiltonian along tempered leapfrog trajectory.

Molecular Dynamics Configuration Evolution $\alpha = 1.01$

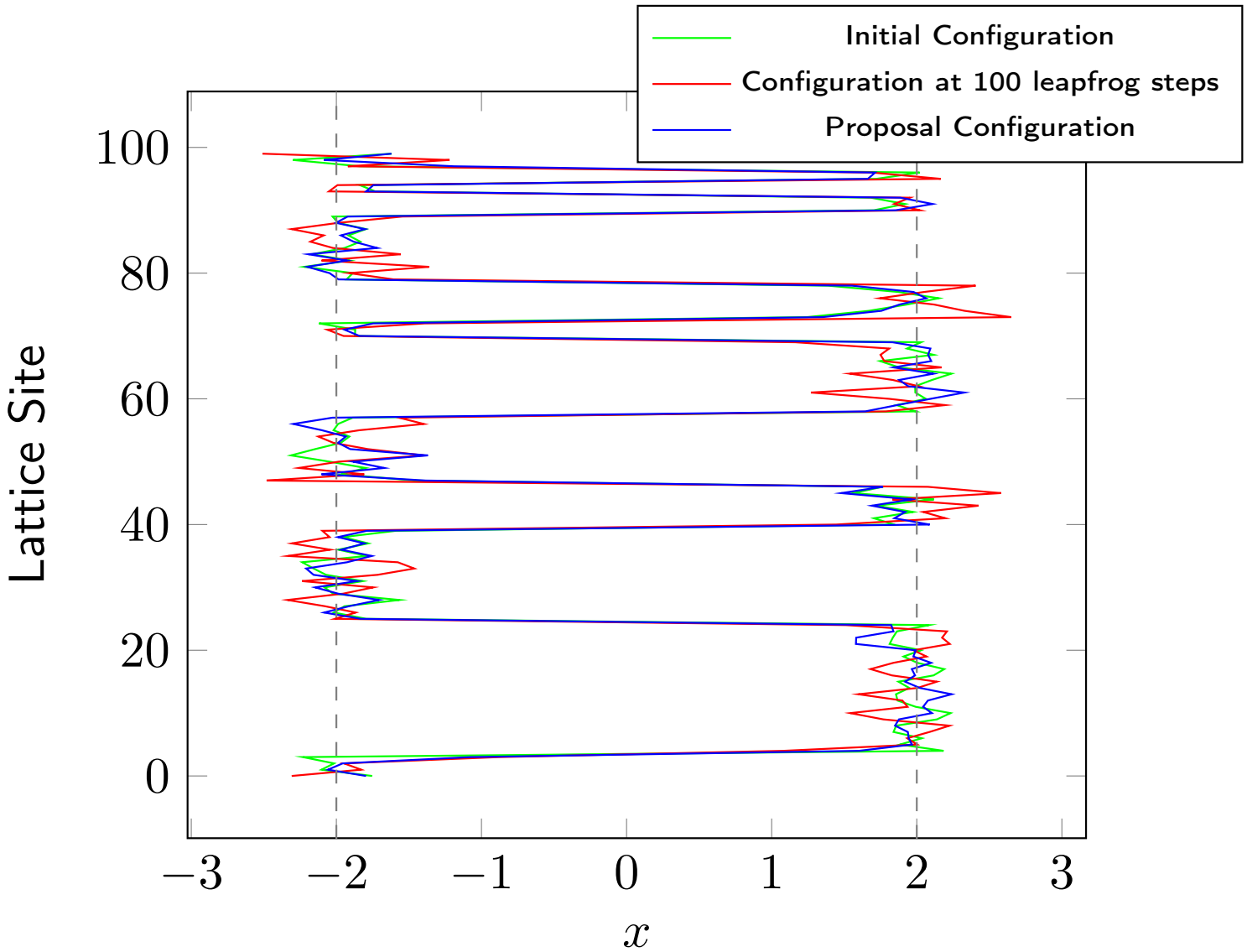

Figure 17: Evolution of the equilibrium configuration along the tempered leapfrog trajectory.

Molecular Dynamics Hamiltonian Evolution $\alpha = 1.05$

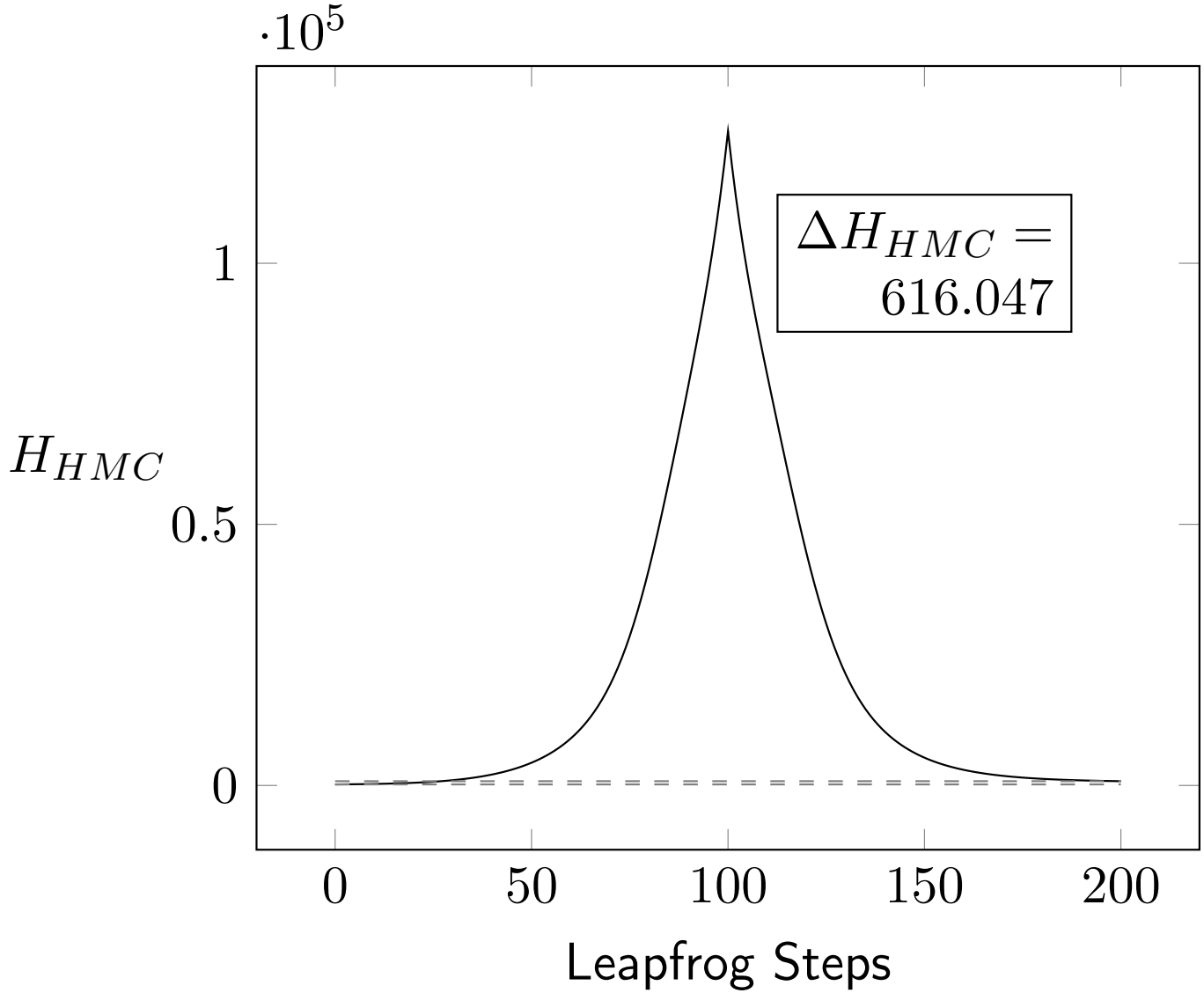

Figure 18: Evolution of HMC Hamiltonian along tempered leapfrog trajectory.

Molecular Dynamics Configuration Evolution $\alpha = 1.05$

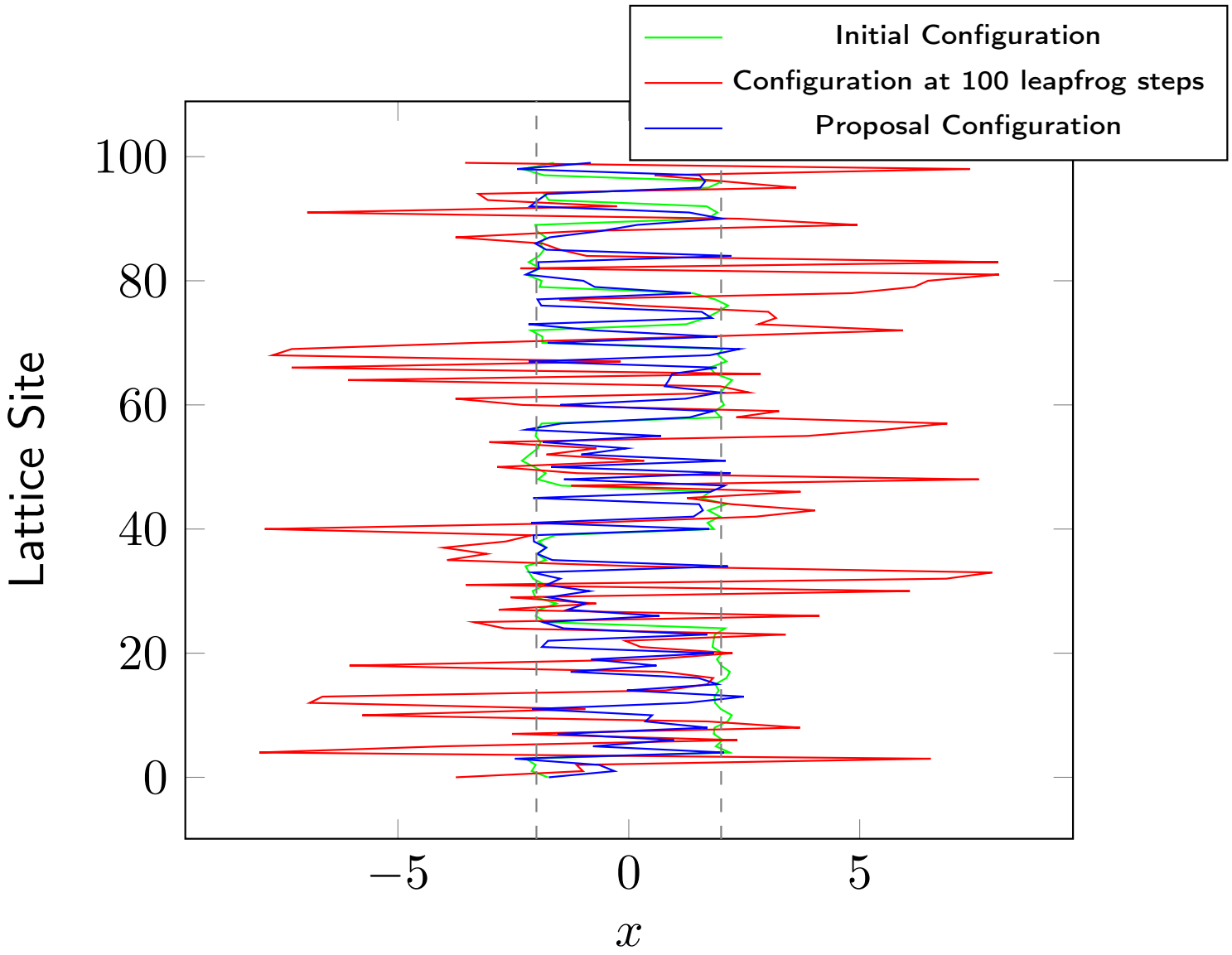

Figure 19: Evolution of the equilibrium configuration along the tempered leapfrog trajectory.

Conclusion

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

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  - 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:

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

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

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:

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

$$J_p = \det \begin{pmatrix} \delta_{ij} & 0 \\ -\epsilon \partial_{q_i} \partial_{q_j} U(\boldsymbol{q}) & \delta_{ij} \end{pmatrix} = 1.$$

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:

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

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

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

Volume Preservation on Phase Space with Tempering II

Jacobians of these mappings:

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

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

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

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:

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

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

Ground State Expectation Values I

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

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

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

Limit that $\tau_b - \tau_a \to \infty$ 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:

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

so for harmonic oscillator:

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

and anharmonic oscillator:

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