Accelerated 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 harmonic and enharmonic oscillator properties.
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  - Can be used for calculations in lattice field theory.

Theory - The Path Integral

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Transition Amplitude

$$\langle x_b, t_b | x_a, t_a \rangle = \int_{x_a}^{x_b} \mathcal{D}x \exp\left({}^{iS[x(t)]}/_{\hbar} \right) \tag{1}$$

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Minkowski Action

$$S_M = \int_{t_a}^{t_b} dt \left[\frac{1}{2} m \left(\frac{dx}{dt}\right)^2 - V(x)\right] \tag{3}$$

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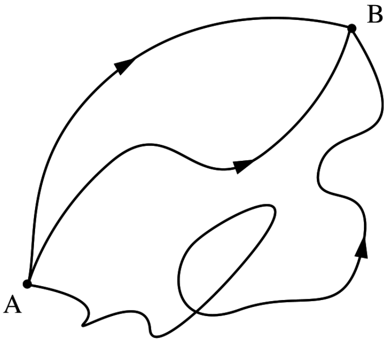

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[1] The Free Encyclopedia Wikipedia. *Path Integral Formulation*. 2017. URL: https://en.wikipedia.org/wiki/Path_integral_formulation#/media/File:Three_paths_from_A_to_B.png.

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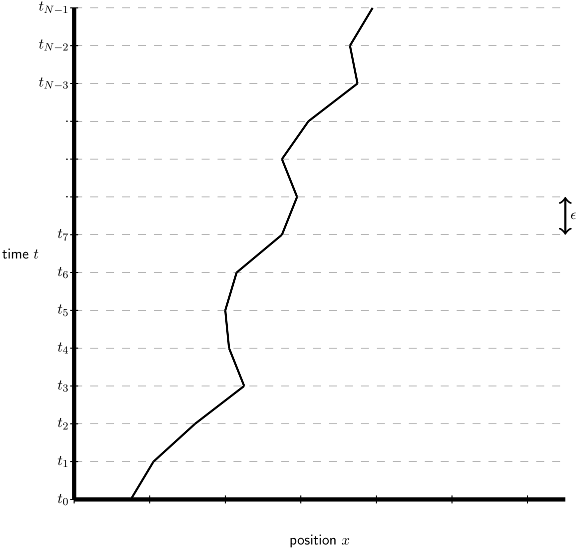

Theory - Discrete Time Lattice

Discrete Action

$$S_M = \sum_{j=0}^{N-1} \epsilon \left[\frac{1}{2} m \left(\frac{x_{j+1} - x_j}{\epsilon} \right)^2 - V\left(x_j\right) \right] \tag{1}$$

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Discrete Path Integral

$$\langle x_b, t_b | x_a, t_a \rangle \sim \int_{-\infty}^{\infty} \prod_{j=1}^{N-1} dx_j \exp\left(\frac{i}{\hbar} S_M \left\{x_j\right\} \right) \tag{2}$$

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Discrete Euclidean Action

$$S_M = i \sum_{j=0}^{N-1} a \left[\frac{1}{2} m \left(\frac{x_{j+1} - x_j}{a} \right)^2 + V\left(x_j\right) \right] := iS_E \tag{5}$$

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Partition Function

$$Z \sim \int_{-\infty}^{+\infty} \prod_{j=1}^{N-1} dx_i \exp\left(-\beta H\left(\left\{x_i\right\}\right)\right) \tag{4}$$

Numerics - Monte Carlo

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Monte Carlo Estimate

$$\bar{A} = \frac{1}{M} \sum_{\nu=1}^{M} A\left(\boldsymbol{x}_{\nu}\right) \tag{5}$$

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Boltzmann Distribution

$$p\left(\boldsymbol{x}_{\nu}\right) \mathcal{D}\boldsymbol{x} = \frac{\exp\left(-S\left(\boldsymbol{x}_{\nu}\right)\right) \mathcal{D}\boldsymbol{x}}{\int \mathcal{D}\boldsymbol{x} \exp\left(-S\left(\boldsymbol{x}\right)\right)} \tag{6}$$

Numerics - Hybrid Monte Carlo Algorithm

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Fictitious Momenta

$$p_i, i = 0 \dots N - 1 \qquad (7)$$

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HMC Hamiltonian

$$H_{hmc} := \sum_{i=0}^{N-1} \frac{p_i^2}{2m} + S\left(\{x_i\}\right) \tag{8}$$

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4. Return to step 1.

Results - Harmonic Oscillator Expectation Values

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Value	Measured	Discrete Theory[1]	Continuum Theory
$\langle x \rangle$	$0.00015(20)$	0	0

[1] M Creutz and B Freedman. "A statistical approach to quantum mechanics". In: *Annals of Physics* 132.2 (1981), pp. 427–462. DOI: 10.1016/0003-4916(81)90074-9.

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$\langle x^2 \rangle$	$0.44723(14)$	0.4472135955	0.5

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E_1	$0.9679(90)$	$FILL$	1

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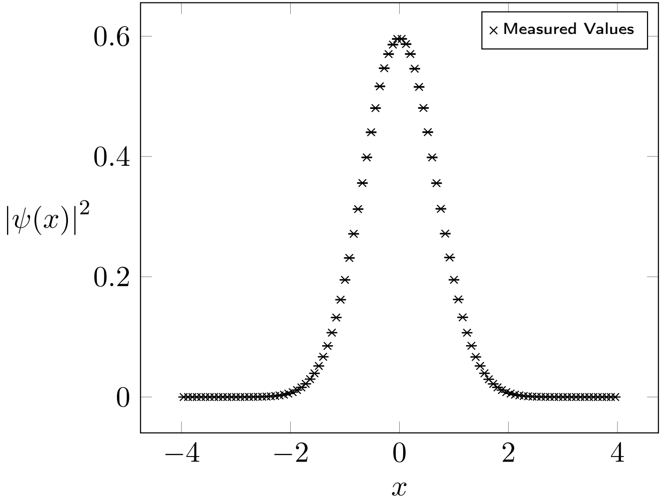

Results - Harmonic Oscillator Wave Function

Discrete Wave Function[1]

$$\psi_{disc.}(x) = \left(\frac{\omega}{\pi}\right)^{\frac{1}{4}} \exp\left(-\frac{1}{2}\omega x^2\right) \tag{7}$$

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$$\omega^2 = \mu^2 \left(1 + \frac{a^2\mu^2}{4}\right) \tag{8}$$

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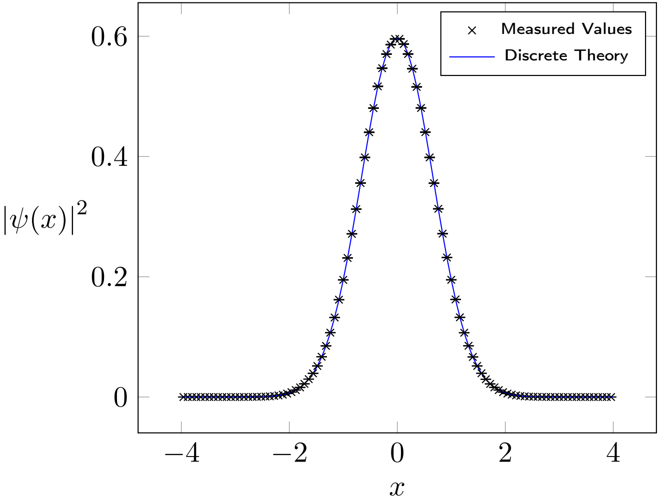

Results - Harmonic Oscillator Wave Function

Continuous Wave Function

$$\psi_{cont.}(x) = \left(\frac{\mu}{\pi}\right)^{\frac{1}{4}} \exp\left(-\frac{1}{2}\mu x^2\right) \tag{7}$$

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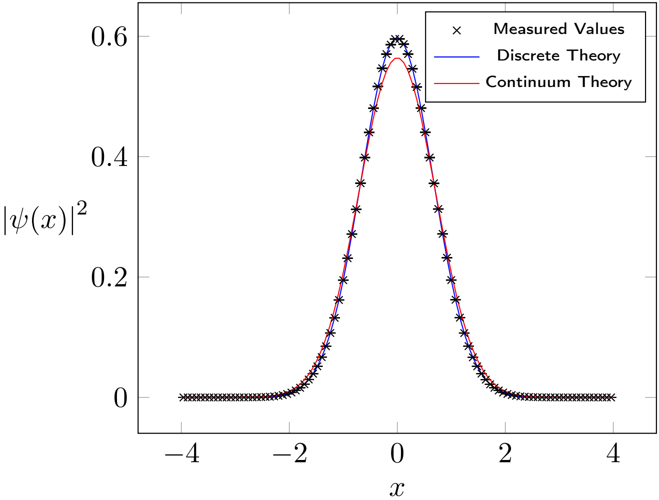

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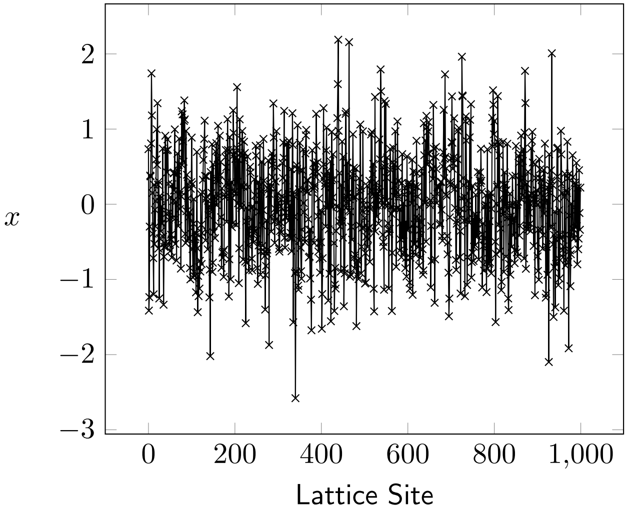

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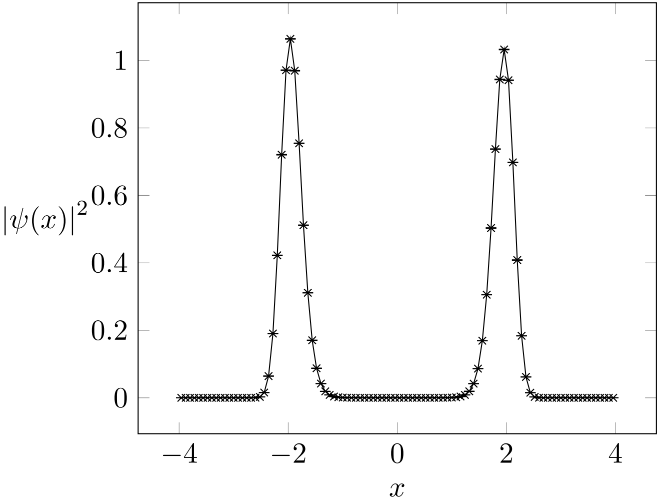

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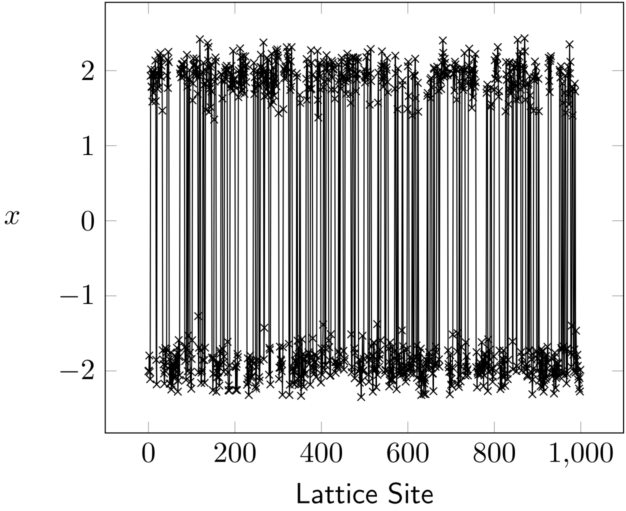

Results - Isolated Modes Wave Function

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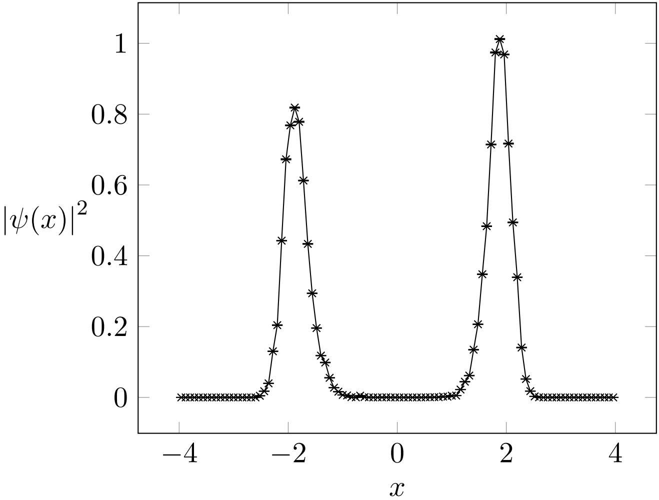

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- Applications of tempering?
  - Potentially applicable to lattice field theory where computation time is far more costly.