Harmonic and Anharmonic Oscillator with Path Integrals

Monte Carlo on the Lattice

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A fundamental problem

- Make calculations of observables for the one dimensional Simple Harmonic Oscillator
- Use Path Integral Formulation on a discrete Euclidean time lattice
- But analytic solution to the Harmonic Oscillator exists, so why bother?
- Go from the Harmonic Oscillator to the *Anharmonic* Oscillator - the basis for a free scalar field theory, the simplest of the quantum field theories.

Path integral formulation

- Deriving **transition probability amplitude** for particle in potential V will lead to the **pathintegral**
- **One-dim. oscillators**:
  Transit. prob. amplitude for change from initial into final state

$$K(x_i, t_i; x_f, t_f) = \langle x_f | \underbrace{e^{-\frac{i}{\hbar}\hat{H}(t_f - t_i)}}_{=U} | x_i \rangle$$

$\hat{H} \triangleq$ One-dim. oscillator Hamiltonian

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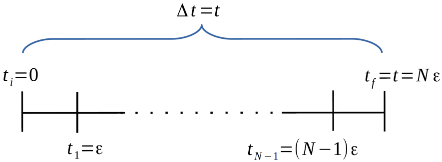

Figure : Division of $[0, t]$ into N equidistant points with distance ϵ

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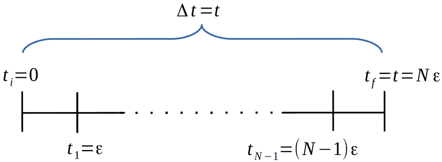

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\begin{aligned}
K(x_i, 0; x_f, t) &= \langle x_f | \, e^{-\frac{i}{\hbar}\hat{H}t} \, | x_i \rangle \\
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- Numerical evaluation: Introduce imaginary time $\tau = it$:

$$e^{i\frac{S}{\hbar}} \rightarrow e^{-\frac{S_E}{\hbar}} = \exp\left(-\frac{a}{\hbar}\sum_{k=1}^{N}\frac{m}{2}\cdot\frac{(x_k - x_{k-1})^2}{a^2} + V(x_k)\right) \tag{1}$$

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  $\Rightarrow$ express expectation values in terms of S_E:

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  - $\boldsymbol{x}_k$ sampled with equilibrium-probab. $P^{eq}(\boldsymbol{x}_k) = \exp\left(-S_E(\boldsymbol{x}_k)/\hbar\right)$

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- How can be ensured that generated paths follow required Boltzmann-distribution?
  - $\Rightarrow$ Implementation of Importance Sampling by generating N config. $\boldsymbol{x}_k$ by means of **Markov Process**
- **Markov chain** is described by PDF $W(x_i, x_f) \geq 0$ for transition $x_i \rightarrow x_f$

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Implementation of oscillator physics

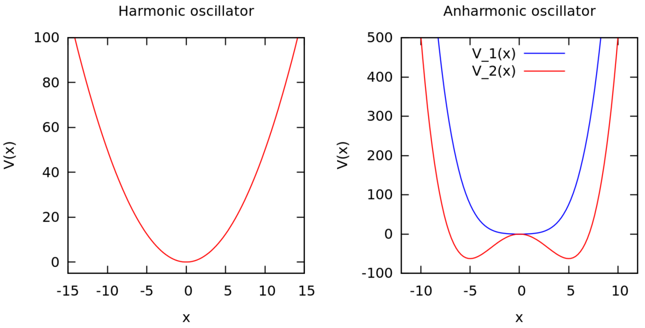

Figure : Lefthand: h.o. potential with $\mu^2 = 1$. Righthand: a.o. potential $V_1(x)$ with $\mu^2 = 1,\ \lambda = 0.1$ and $V_2(x)$ with $\mu^2 = -10,\ \lambda = 0.1$.

$$V(x) = \frac{1}{2} m\omega^2 x^2 + \lambda x^4 = \frac{1}{2}\mu^2 x^2 + \lambda x^4$$

Groundstate energy

$$\langle \hat{H} \rangle (t) = \frac{\sum_{x=0}^{n} \langle x | e^{-\beta \hat{H} t} \hat{H} | x \rangle}{\sum_{x=0}^{n} \langle x | e^{-\beta \hat{H} t} | x \rangle} \approx \frac{E_0 e^{-\beta E_0 t}}{e^{-\beta E_0 t}} = E_0$$

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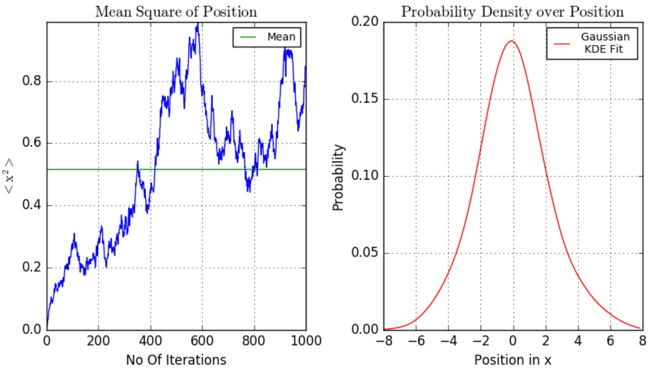
The Approach

- MCMC is carried out on a 1-D discrete time lattice with a spacing a.
- A path is generated by either random sampling - a hot start or all the values of the path are 0.0 - a cold start.
- With the path generated, the burn-in phase is passed with a thermalization run of several Monte Carlo iterations.
- Once equilibrium is reached, a meaningful extraction of observables and properties can be made.


Mean Square of Position
Mean
$<x^2>$
0.0
0.2
0.4
0.6
0.8
0
200
400
600
800
1000
No Of Iterations
Probability Density over Position
Gaussian
KDE Fit
Probability
0.00
0.05
0.10
0.15
0.20
−8
−6
−4
−2
0
2
4
6
8
Position in x

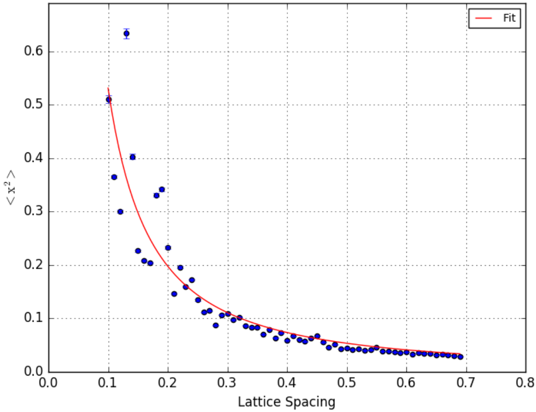
Mean Square Position

- The first meaningful observable that was measured and worked on here was the mean square position.
- The observable showed an increase to a certain value after which the observable merely showed statistical fluctuations around this mean value.
- This value can be compared to the one obtained from an analytical expression in discrete lattice theory

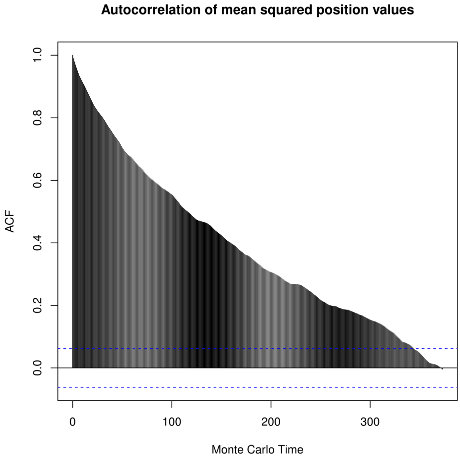
$$\left\langle x^2 \right\rangle = \frac{1}{2\mu(1+a^2\mu^2/4)^{1/2}} \left(\frac{1+R^N}{1-R^N} \right) \tag{6}$$

where $R = 1 + a^2\mu^2 - a\mu(1 + a^2\mu^2/4)^{1/2}$

Mean Square Position



Autocorrelation of Monte Carlo Estimates



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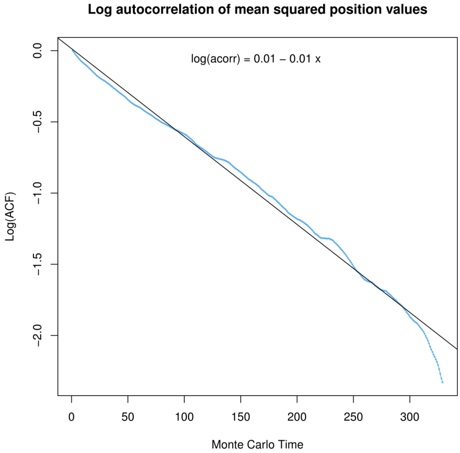
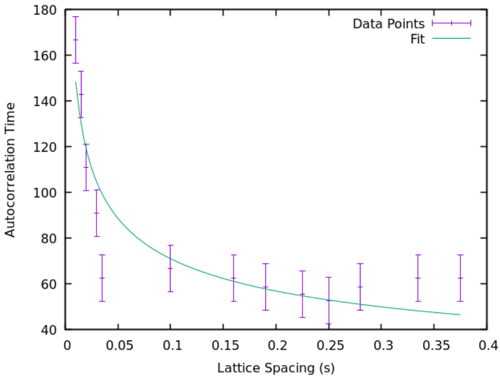


Autocorrelation Time



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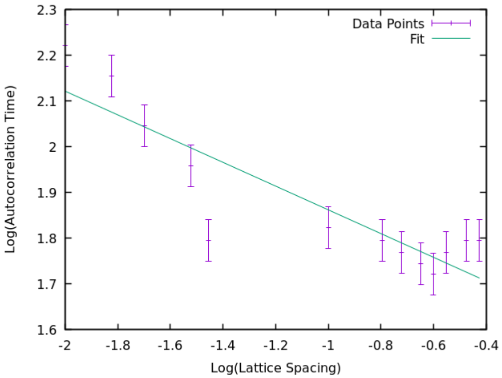
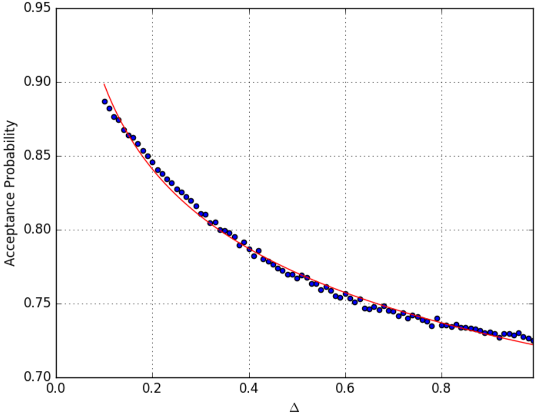
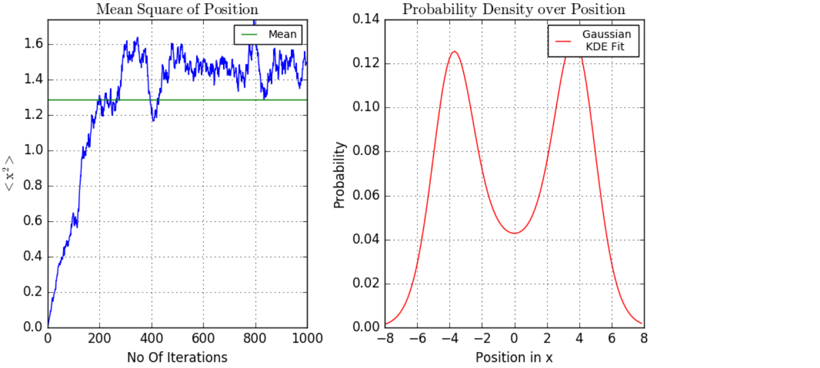


Optimizing Δ



The potential was modified to bring about the anharmonicity as:

$$V(x) = \lambda(x^2 - f^2)^2 \tag{7}$$



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Literature

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Thanks for your attention.

Ground State Energy of the Anharmonic Oscillator