Lattice Monte Carlo Study of the Harmonic Oscillator in the Path Integral Formulation

DESY Summer Student Programme - Zeuthen 2012

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Introduction - A bit of theory

- From Operators to the Path Integral
- Connection With Statistical Mechanics

Numerical Approach to Evaluate Path Integrals

- Numerical Approach
- Metropolis Algorithm
- Statistical and Systematic Error Effects in the System

Results

- Ground Energy for The Harmonic Oscillator
- Energy of the First Excited for the Harmonic Oscillator

Summary

- Analytical Results for the Harmonic Oscillator

From Operators to the Path Integral

- Problem: evaluate $\langle x_F|e^{-iHT}|x_I\rangle$
- Discretize time: $T = N\delta t$
  - $\langle x_F|e^{-iHT}|x_I\rangle = \langle x_F|e^{-iH\delta t}e^{-iH\delta t}\dots e^{-iH\delta t}|x_I\rangle$
- Use completeness relation $\int dx|x\rangle\langle x| = 1$ between each operator

$$\langle x_F|e^{-iHT}|x_I\rangle = \left(\prod_{i=1}^{N-1}\int dx_i\right)\langle x_F|e^{-iH\delta t}|x_{N-1}\rangle\langle x_{N-1}|e^{-iH\delta t}\dots e^{-iH\delta t}|x_1\rangle\langle x_1|x_I\rangle$$

- Evaluate $\langle x_{i+1}|e^{-iH\delta t}|x_i\rangle$
  - $\frac{1}{2\pi}dp \int |p\rangle\langle p| = 1$
  - $H = \frac{p^2}{2m} + V(x)$
  - $\langle x|p\rangle = e^{ipx}$
  - $e^{iT\delta t + iV(x)\delta t} = \ldots e^{\frac{i}{2}\delta t[T,H]} e^{iT\delta t} e^{iV(x)\delta t} \cong e^{i\delta t T} e^{i\delta t V(x)}$
- Final result: Gaussian Integral
  - $\langle x_{i+1}|e^{-iH\delta t}|x_i\rangle = \frac{e^{-i\delta t V(x_{i+1})}}{2\pi} \int dp \exp\left[-i\delta t \frac{p^2}{2m} + ip(x_{i+1} - x_i)\right]$
- Complete squares
  - $\langle x_{i+1}|e^{-iH\delta t}|q_i\rangle = \left(\frac{-im}{2\pi\delta t}\right)^{1/2} \exp\left\{i\delta t\left[\left(\frac{x_{i+1}-x_i}{\delta t}\right)^2 - V(x_{i+1})\right]\right\}$
- We use this to rewrite $\langle x_F|e^{-iHT}|x_I\rangle$

Time to go the continuum limit!

That means, keeping $T = Na = \text{const.}$, we take the limit of $N \to \infty$ and $a \to 0$

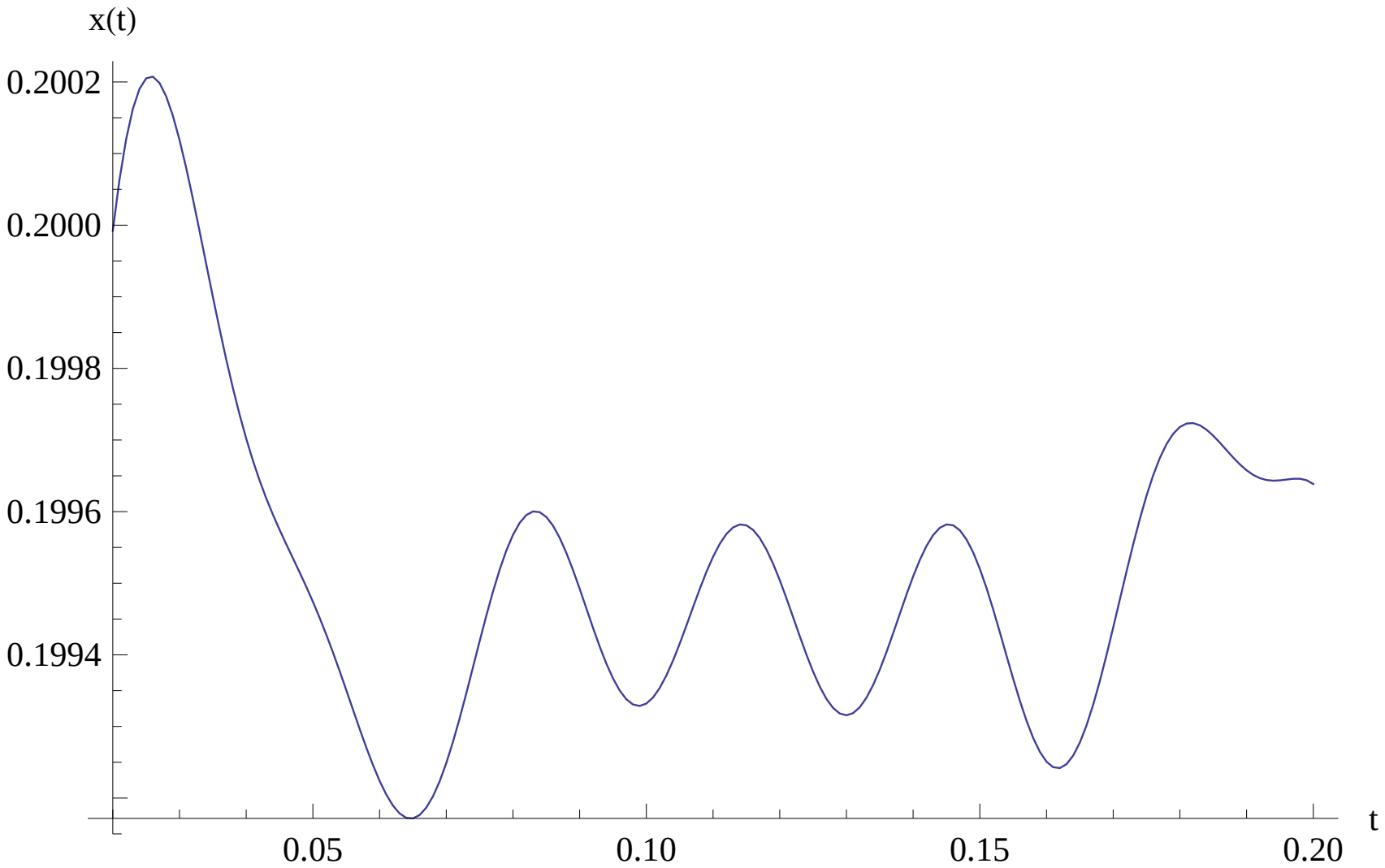
$$\left(\frac{-im}{2\pi a}\right)^{\frac{N-1}{2}} \left(\prod_{i=1}^{N-1} \int dx_i\right) \to \int \mathcal{D}[x(t)],$$

$$\frac{x_{j+1} - x_j}{a} \to \dot{x},$$

$$a \sum_{j=0}^{N-1} \to \int dt,$$

We arrive then at the path integral formulation for Quantum Mechanics

$$\langle x_F | e^{-iHT} | x_I \rangle = \int \mathcal{D}[x(t)] \exp\left[i \int dt \frac{m\dot{x}^2}{2} - V(x)\right] = \int \mathcal{D}[x(t)] e^{iS[x(t)]}$$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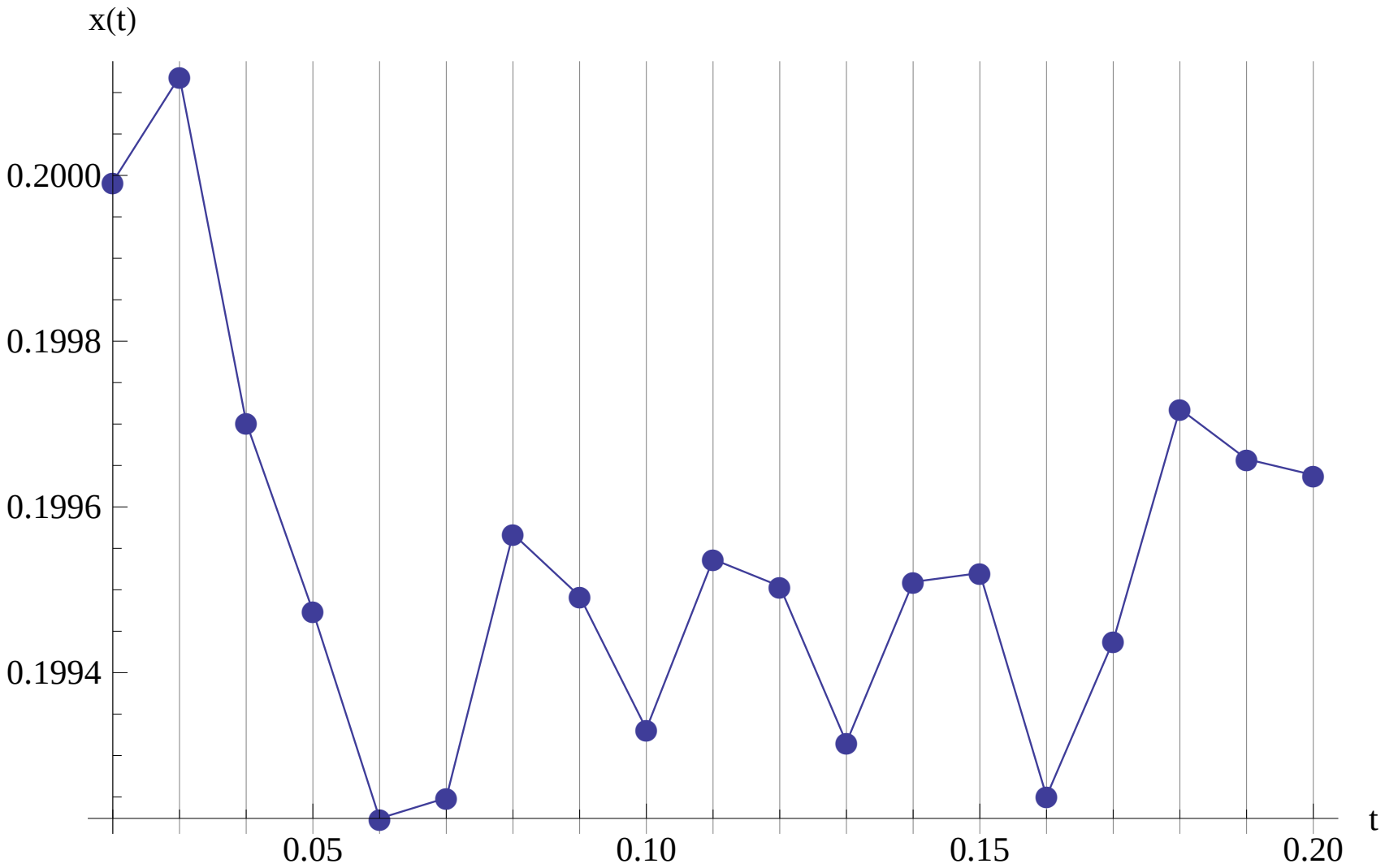
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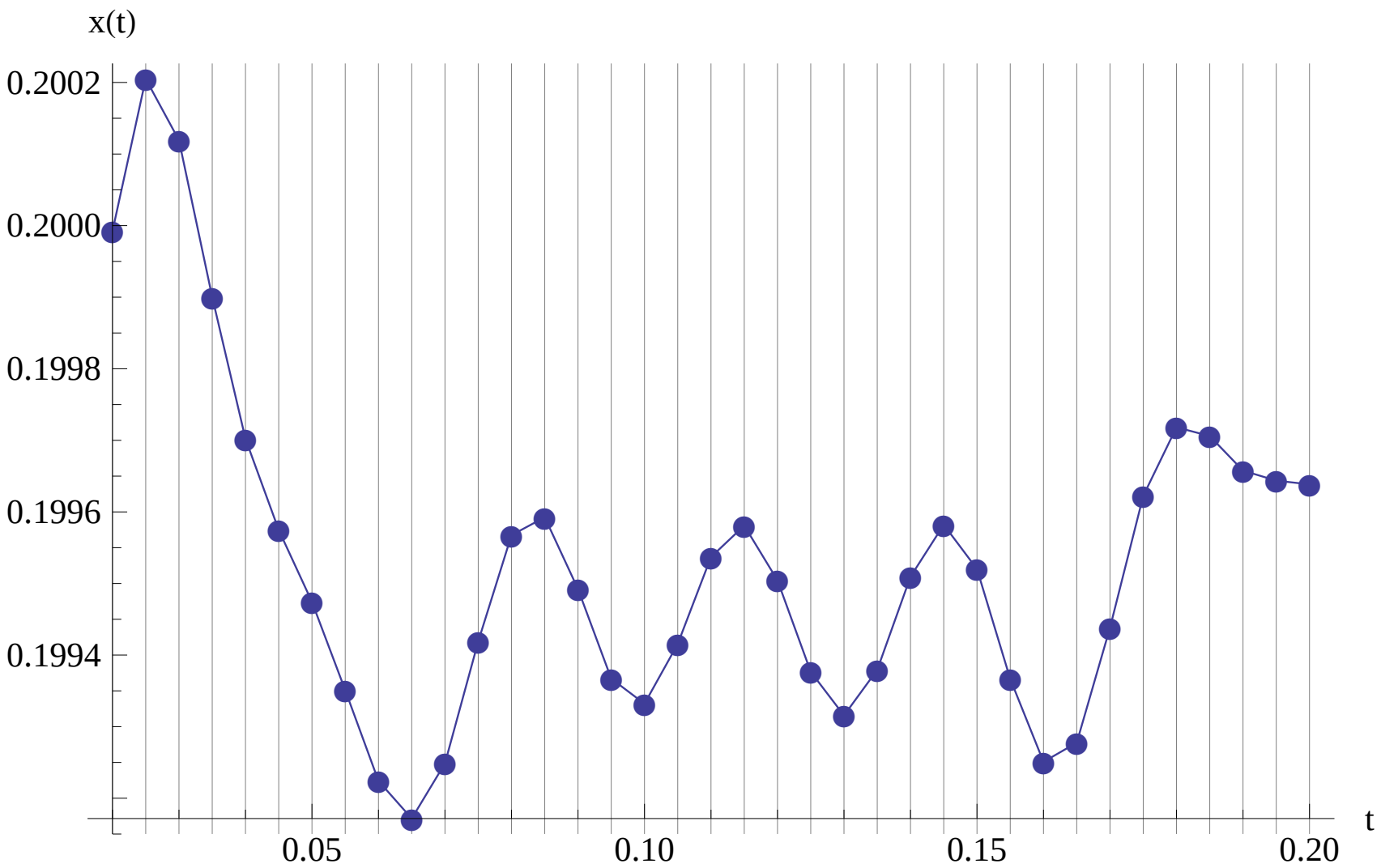
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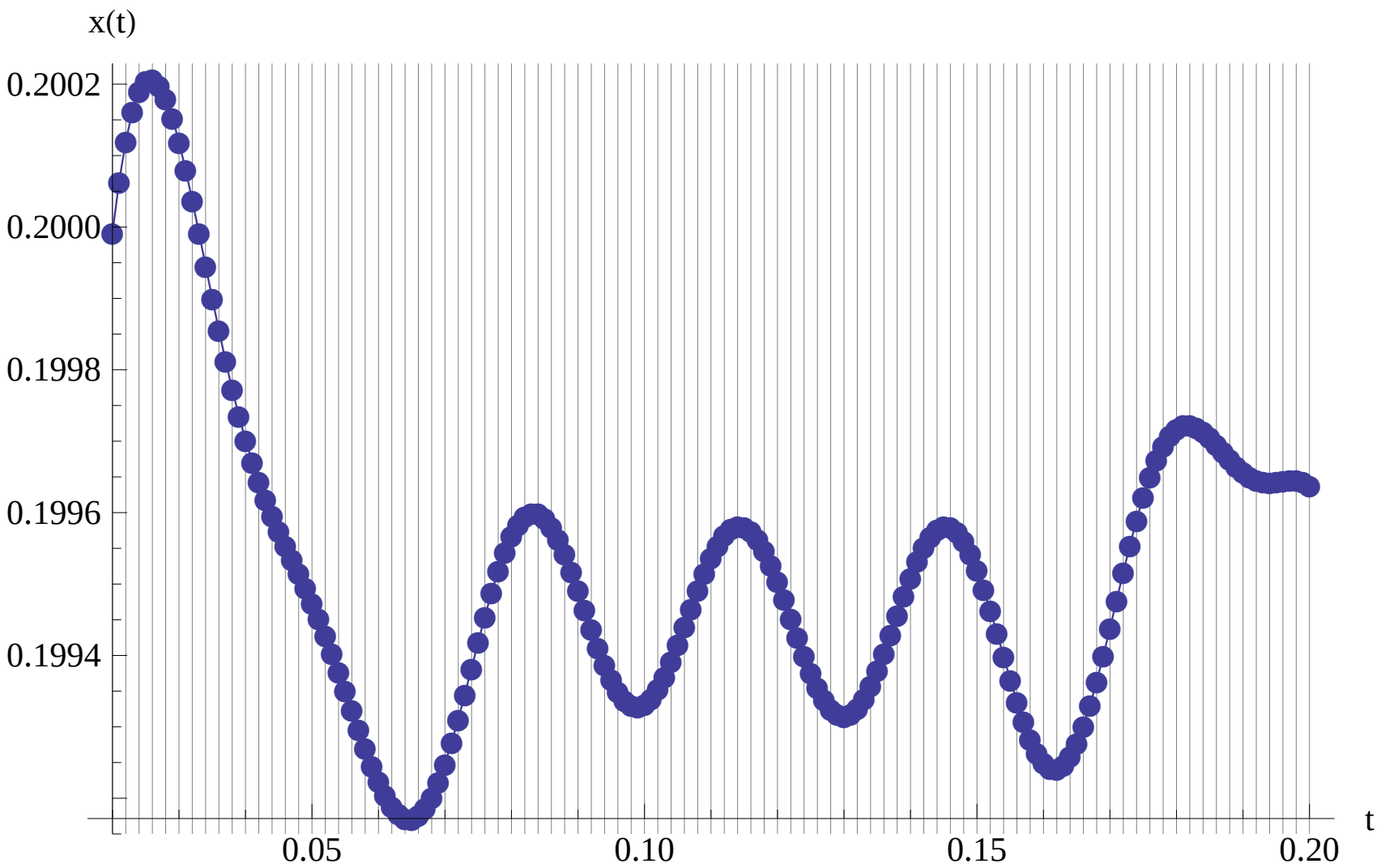
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Connection With Statistical Mechanics

- Step back to discretized time
- Transform to Euclidean time: $t \rightarrow -it$
- Same integral as the partition function!

$$Z \propto \int e^{[-\beta H(p_1,p_2,\ldots,p_N,x_1,x_2,\ldots,x_N)]}\, d^3p_1\, d^3p_2 \ldots d^3p_N\, d^3x_1\, d^3x_2 \ldots d^3x_N$$

$$\beta = \frac{1}{k_b\theta}$$

$$Z_{FI} = \left(\frac{-im}{2\pi\delta t}\right)^{\frac{N-1}{2}} \left(\prod_{i=1}^{N-1} \int dq_i\right) \exp\left[-\delta t \sum_{j=0}^{N-1} \left(\frac{x_{j+1}-x_j}{\delta t}\right)^2 + V(x_{j+1})\right]$$

- Expectation value of an operator $\hat{A}$

$$\langle \hat{A} \rangle = \mathrm{Tr}[e^{-HT}\hat{A}]/Z = \langle \hat{A} \rangle = \frac{\left(\prod_{i=0}^{N} \int dx_i\right) A(x_1, x_2, \ldots, x_n) e^{-S[x(t)]}}{\left(\prod_{i=0}^{N} \int dx_i\right) e^{-S[x(t)]}}$$

- Apply completeness relation for energy states $\sum_{n=1}^{M} |n\rangle\langle n| = 1$ and the limit $T \to \infty$
  - In our analogy with Statistical Physics, this is equivalent for taking the limit of zero temperature
- We conclude that in this limit $\langle \hat{A} \rangle = \langle 0|\hat{A}|0\rangle$
- The ground state energy is given by

$$E_0 = \lim_{T\to\infty} \langle \hat{H} \rangle = \frac{\left(\prod_{i=0}^{N} \int dx_i \left[x_i V'(x_i)/2 + V(x_i)\right] e^{-S[x(t)]}\right)}{\left(\prod_{i=0}^{N} \int dx_i\right) e^{-S[x(t)]}}$$

Remark: We used the Virial Theorem here: $\langle E_{kin} \rangle = \langle xV'(x) \rangle /2$

- n-point connected propagator

$$\Gamma_c^{(n)} = \prod_{i=1}^{n} \frac{\partial}{\partial J_i} \ln\left[Z(J)\right]\Big|_{J=0}$$

$$Z(J) = \mathrm{Tr}\left[\exp\left(-HT + \sum_{k=1}^{n} x_k J_k\right)\right]$$

- For $n = 2$ and $T \to \infty$

$$\Gamma_c^{(2)}(\tau) = \langle 0|x(0)x(\tau)|0\rangle - \langle 0|x(0)|0\rangle\langle 0|x(\tau)|0\rangle$$

- Using again the completeness relation, changing to the Schrödinger representaion ($x(\tau)_H = e^{-H\tau} x_S e^{H\tau}$) and taking the limit $\tau \to \infty$

$$\Gamma_c^{(2)}(\tau \to \infty) = |\langle 0|x|1\rangle|^2 \, e^{-(E_1 - E_0)\tau}$$

Numerical Approach

We applied **Metropolis algorithm** to generate random paths between initial and final position of the particle. Instead of random sampling we based on **importance sampling**, which is sampling from a given distribution.

We considered a Boltzmann distribution with the action S treated as a factor.

$$P(x) \sim \exp[-S(x)]. \tag{1}$$

The expected value of any observable A is given by the expression

$$\langle A \rangle = \frac{1}{Z} \int A(x) \exp[-S(x)] \mathcal{D}x, \tag{2}$$

where $Z = \int \exp[-S(x)] \mathcal{D}x$ is the partition function.

Main Idea of our Computations

We need to find the way of generating random points x_i with the distribution

$$P(x) = \frac{\exp\left[-S(x)\right]}{\int \exp\left[-S(x)\right]\mathcal{D}x}, \tag{3}$$

which will lead us to obtain the Monte Carlo estimate of the expectation value $\langle A \rangle$

$$\langle A \rangle = \frac{1}{N_{path}} \sum_{i=1}^{N_{path}} A(x_i), \tag{4}$$

where N_{path} is the number of paths generated with Metropolis Algorithm. Because N_{path} is a finite number, a statiscal error occurs. We are going to discuss it later.

Metropolis Algorithm

Suppose that:

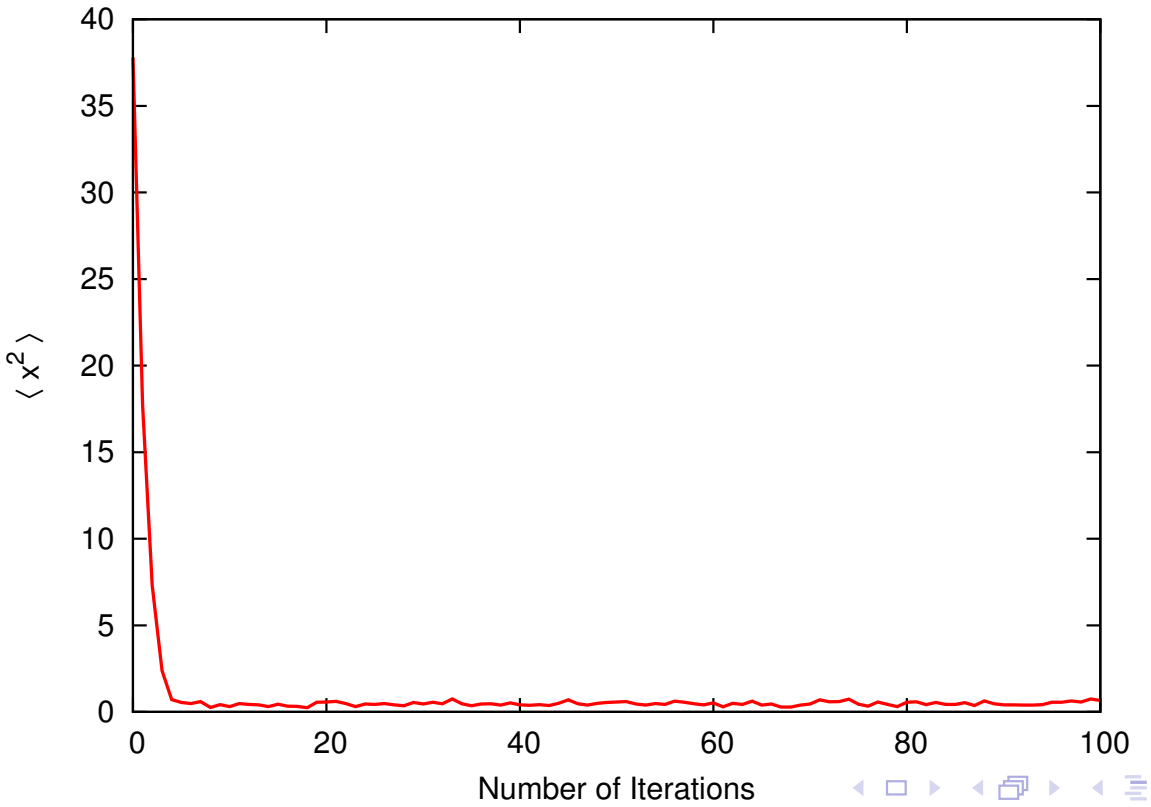
- $S(x)$ is the action of the given system,
- Δ_x is an algorithm parameter,
- x is a set of points representing coordinates in quantum mechanics (fields in quantum field theory)
- N is the number of points on our time lattice and therefore number of the particle path's coordinates as well.

1. Generate any **random path** $x = (x_1, x_2, \ldots x_N)$ between initial and final position of the particle.
2. Choose the random point x_i' with uniform probability within the interval
$$[x_i - \Delta_x, x_i + \Delta_x].$$
3. Replace point x_i with new value x_i' and calculate the difference in the action
$$\Delta S(x_i', x_i) := S(x_i') - S(x_i).$$
4. If $\Delta S(x_i', x_i) < 0$, then accept x_i' point and change initial path.
5. If $\Delta S(x_i', x_i) \geq 0$, then generate random number r within $[0, 1]$.
   - If $\exp[-\Delta S(x_i', x_i)] > r$, then accept x_i' point and change initial path.
   - Otherwise, reject x_i' and apply algorithm for the next point of initial path.

This algorithm fullfills detailed balance

Thermalization

In order to get the proper sample of path's points x_i, we have to generate several trajectories using given algorithm. Statistical calculation can be done only after thermalization point is reached.



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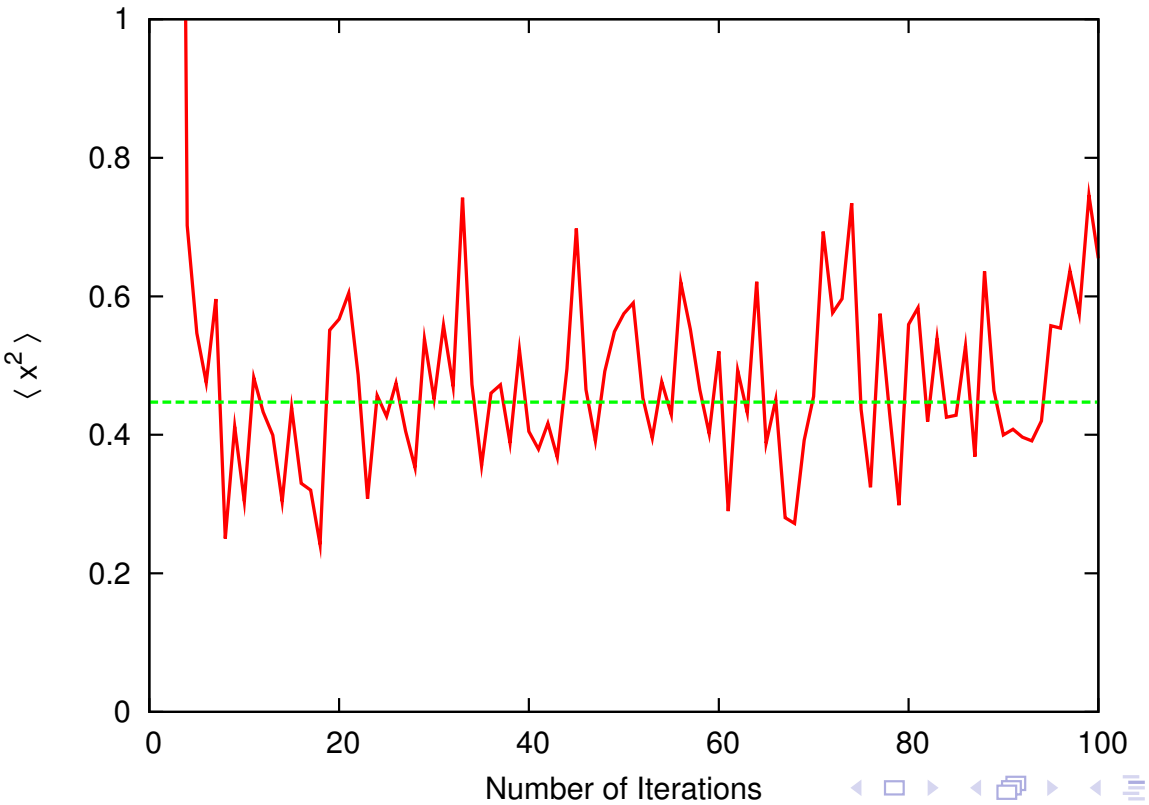


Statistical and Systematic Error Effects in the System

There can appear some systematic effects due to the pseudo-random mechanism and to the fact that the new coordinate depends on the old one. We observe correlation between different paths and its impact on expectated values. There are some statistical dependencies between different configurations. To describe how similar two functions or sequences are we define **correlation function**:

$$C_{ij}(s, s') = corr(X_i(s), X_j(s')), \tag{5}$$

where *corr* is given by the expression

$$corr(X, Y) = \rho_{X,Y} = \frac{\langle (X - \langle X \rangle)(Y - \langle Y \rangle) \rangle}{\sigma_X \sigma_Y}. \tag{6}$$

σ_X and σ_Y are standard deviations for expected value of X and Y.

Correlation

Correlation function for our algorithm is claimed to have an exponential decay of the form

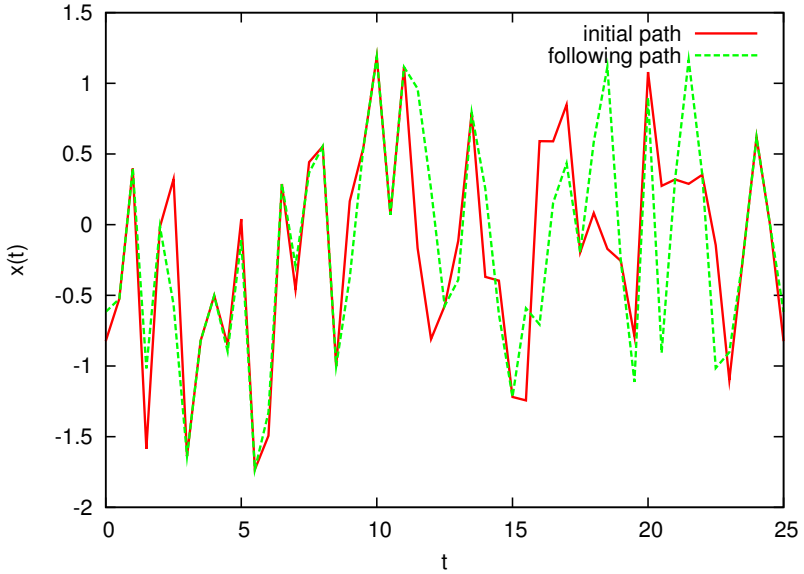
$$C(t_{N_{Paths}}) \sim e^{\frac{-t_{N_{Paths}}}{\tau_c}}. \tag{7}$$

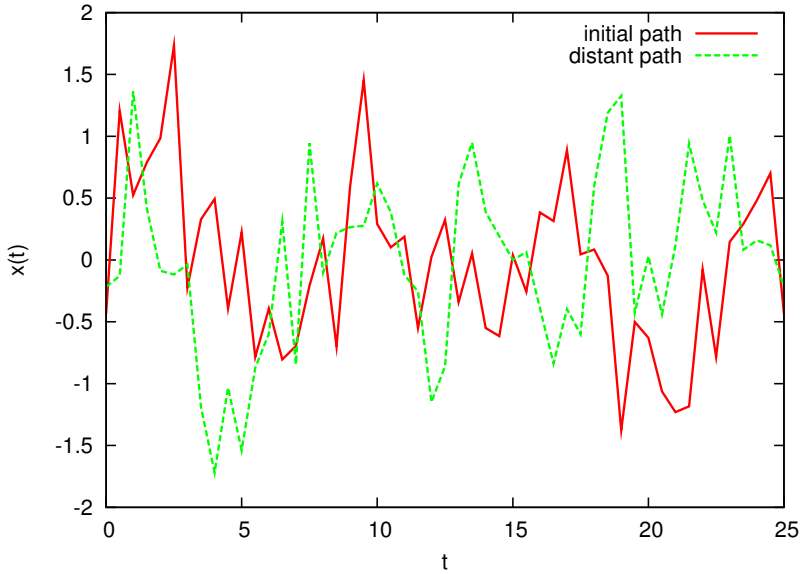
The τ_c parameter is called correlation time and plays the main role in statistical results.

Example. We run our algorithm 100 times and we generate 100 paths.

- If $\tau_c = 1000$, then $C(t_{100}) \sim e^{\frac{-100}{1000}} = e^{-0.1} \approx 0.9$
- If $\tau_c = 1$, then $C(t_{100}) \sim e^{\frac{-100}{1}} = e^{-100} \approx 3.7 \times 10^{-44}$

For long enough time, the position will be no longer closely related to the previous point. Therefore the measurements will become approximatelly independent of each other.





If we let the system wander around for a few system correlation times between measuring samples, the measurements have a good chance of being statistically independent of each other.

Ground Energy for The Harmonic Oscillator

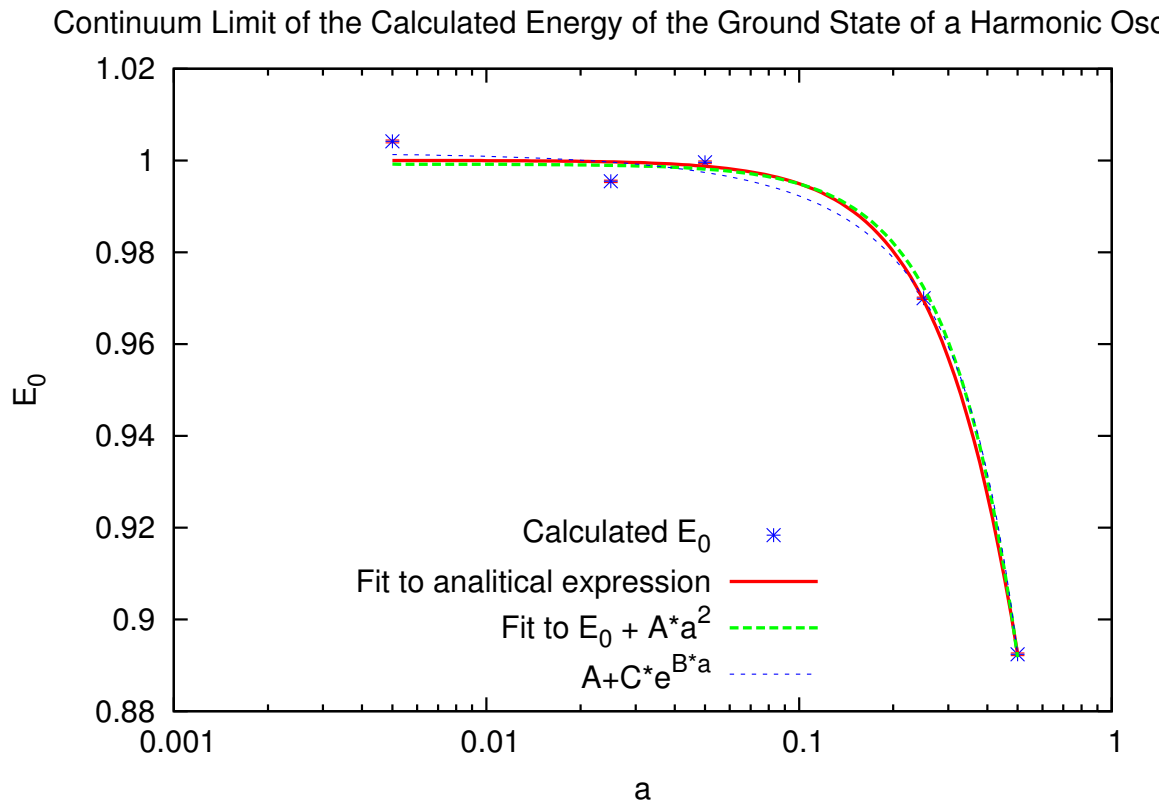
- We will use as the system action

$$S = a\sum_{i=1}^{N} \frac{m}{2}\left(\frac{x_{i+1}-x_i}{a}\right)^2 + \frac{\mu^2 x_i^2}{2} \tag{8}$$

- from Virial theorem $E_0 = \mu^2\langle x^2\rangle$
- $m = 0.5$, $\mu^2 = 2$ and $T = 25$
- First trials with one measurement each 5 Monte Carlo iterations (approximately 20,000 measurements).
  - Results deviated highly from the analytical prediction for small a (possibly high correlation between paths on this limit).
  - For $a = 5 \times 10^{-3}$
    - $E_{0,\text{analytical}} = 0.99999$
    - $E_{0,\text{computed}} = 1.03073 \pm 5.4 \times 10^{-4}$

- Increased for one measurement each 25 Monte Carlo iterations
  - Observed improvement on the results
- For getting the continuum limit, try to fit points to functions
  - $E_0(a) = E_0/\sqrt{1 + Ba^2}$ (Inspired by the analytical solution)
  - $E_0(a) = E_0 + Aa^2$ (Taylor series in a plus assymptotic approach to the continuum value)
  - $E_0(a) = A + Ce^{Ba}$ (ad hoc function)

Ground Energy for The Harmonic Oscillator

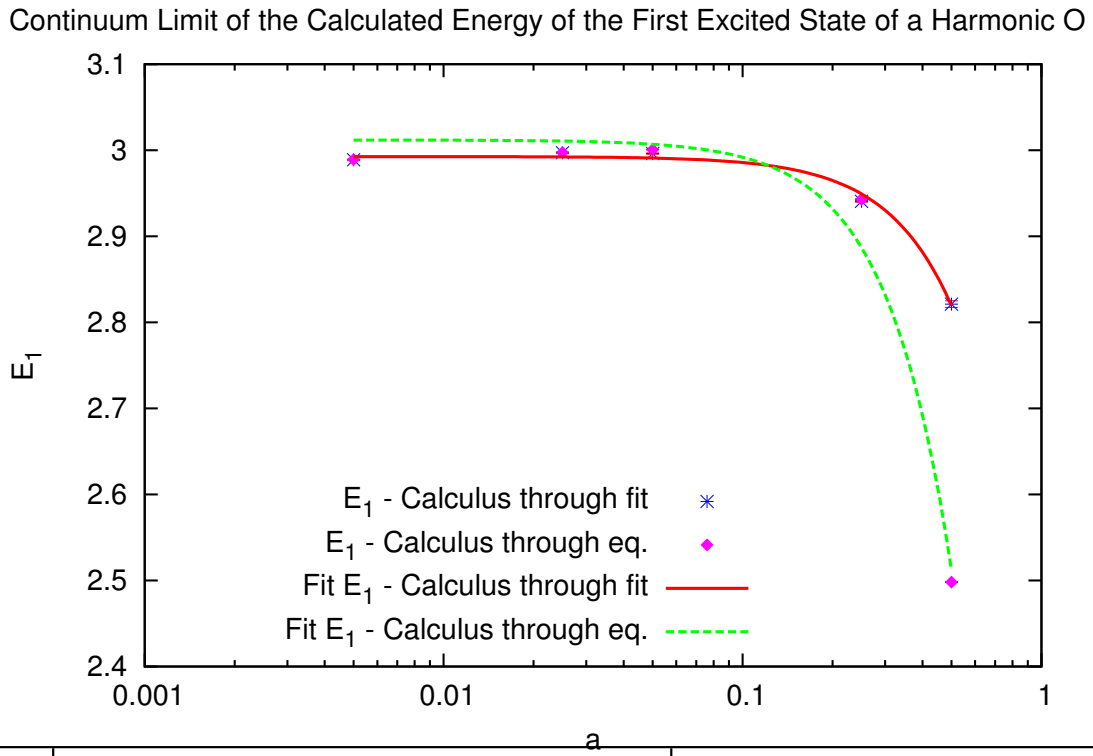


$E_0/\sqrt{1+Ba^2}$	$E_0 + Aa^2$	$A + Ce^{Ba}$ Calculated
$E_0 = 1.000 \pm 0.002$	$E_0 = 0.999 \pm 0.002$	$A = 1.02 \pm 0.01$
$B = 1.02 \pm 0.02$	$A = -0.43 \pm 0.02$	$B = 3.6 \pm 0.8$
		$C = -0.02 \pm 0.01$

Energy of the First Excited for the Harmonic Oscillator

- It is determined in two ways
  - through the formula $E_1 = E_0 - \frac{1}{a} \ln \left[\frac{\langle x_0 x_{i+1} \rangle}{\langle x_0 x_i \rangle} \right]$
  - through the fit of the data into $\Gamma_c^{(2)}(\tau \to \infty) = |\langle 0|x|1\rangle|^2 \, e^{-(E_1 - E_0)\tau}$
- One measurement each 25 Monte Carlo iterations is not good enough
  - $E_{1,\text{analytical}} = 2.99998$
  - $E_{1,\text{computed}} = 2.94124 \pm 6.3 \times 10^{-4}$
- Increase to one measuremnt each 50 iterations
- To get the continuum limit, we adopt the same procedure as E_0: record E_1 as a function of a and fit a function $E_1(a) = E_1 + Ba^2$

Energy of the First Excited for the Harmonic Oscillator



Parameters of the fit	Calculated through fit $e^{-(E_1-E_0)\tau}$	Calculated through $E_1 = E_0 - \frac{1}{a}\ln\left[\frac{\langle x_0 x_{i+1}\rangle}{\langle x_0 x_i\rangle}\right]$
E_1	2.993 ± 0.004	3.01 ± 0.02
B	-0.69 ± 0.03	-2.0 ± 0.17

- Huge disagreement between data for $a = 0.5$
- Two sources of systematic error:
  - Periodic boundary conditions adds growing exponential
  - On practice, we cannot take $\tau \to \infty$ (We use $\tau = 4a$ here)
- Most drastic source of error here is the first one, since the choise of $\tau = a$ improve results
- However for small a the second source of error starts to dominate

So what we actually did in here...?!

- Studied the lattice approach to the path integral formulation of non-relativistic quantum mechanics.
- Adopted Monte Carlo method for calculations of E_0 and E_1 for the harmonic oscillator.
- Observed how the quantum mechanics paths evolve in time.
- Observed how discretized quantum mechanical system approaches the continuum limit.

And finally, what is the most important: **our final results are compatible with the analytical values!**

Acknowledgements

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Also, we would like to say thank you for all summer students colleagues that we met during our stay here for the amazing friendship created here!

Thank you for your attention!!!

Analytical Results for the Harmonic Oscillator

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

$$R = 1 + \frac{a^2\mu^2}{2m} - a\mu\sqrt{\frac{1}{m} + \frac{a^2\mu^2}{4m^2}}$$

$$\langle x_{i+j} x_i \rangle = \frac{R^j + R^{N-j}}{2(1 - R^N)\mu\sqrt{m + \frac{a^2\mu^2}{4}}}$$

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

$$E_1 = E_0 - \frac{1}{a} \ln \left[\frac{R^{j+1} - R^{N-j-1}}{R^j - R^{N-j}} \right]$$