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Harmonic Oscillator with Path Integral Monte-Carlo on the Lattice

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physics760: Computational Physics

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Introduction

- **Path integral method** method is the quantum mechanical generalisation of the **Principle of stationary Action**.
- Harmonic oscillator is well-understood
- Anharmonic oscillator serves as a toy model for the tunnelling effect
- Path-integral formalism used in more interesting systems as the QCD.

Theory

- Transition probability is $K(a, b) = \int_a^b e^{iS/\hbar} \mathcal{D}x(t)$
- $\mathcal{D}x(t)$ means integration over all paths starting at a and resulting in b.
  - Fast oscillations of the phase
  - Infinite dimensional integral over infinite boundaries
    $\Rightarrow$ analytically generally not solvable
- transition into **Euclidean** time $t \to it$, called **Wick**-rotation

Theory

- $S = \tau \sum_i V(x_i) + T(x_i, x_{i+1})$
- only ΔS is important $\Rightarrow$ complete recalculation is not necessary
- $\Delta S = \tau(V(x_{i;new}) - V(x_{i;old}) +$
  $+ T(x_{i-1}, x_{i;new}) + T(x_{i;new}, x_{i+1}) - T(x_{i-1}, x_{i;old}) - T(x_{i;old}, x_{i+1}))$
- Potential energy: $V(x) = \mu x^2 + \lambda x^4$
- Kinetic energy: $T(x_1, x_2) = \frac{m}{2} \frac{(x_1 - x_2)^2}{\tau^2}$

Methods

- Metropolis-Hastings algorithm
- Initialisation of the (time) lattice with for example gaussian distributed random values
- Iterate repeatedly over all lattice sites
- Draw a new value for current lattice site
- Evaluate $\Delta S < 0 \Rightarrow$ accept change
- Else: Accept if $e^{-\Delta S/\hbar} > x$ for $x \in [0, 1]$ evenly distributed

Implementation

- Implemented in Python3
- Main loop implemented in C++ to improve performance drastically
- Plotting done in Python3

Verification: Harmonic oscillator

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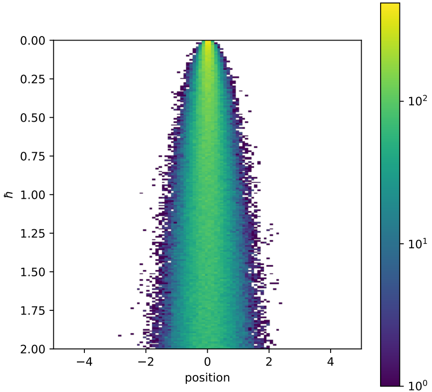
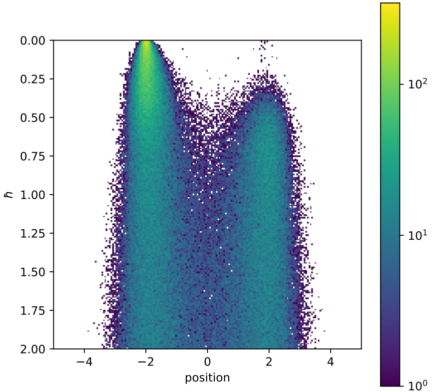


- Condenses into classical minimum for $\hbar \to 0$

Classical limit harmonic oscillator.

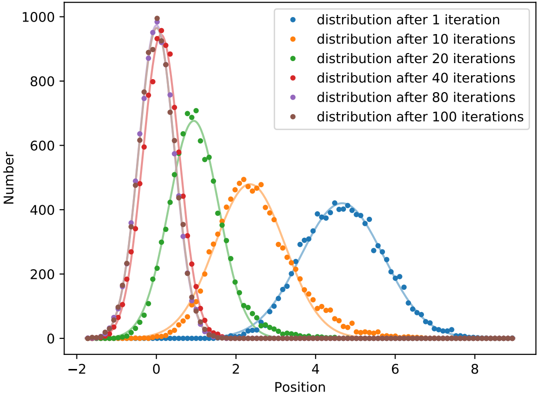
Verification: Anharmonic oscillator



- Initially prepared in the left minimum
- Condenses into classical minimum for $\hbar \to 0$
- For low $\hbar$ right minimum is not populated

Classical limit anharmonic oscillator.

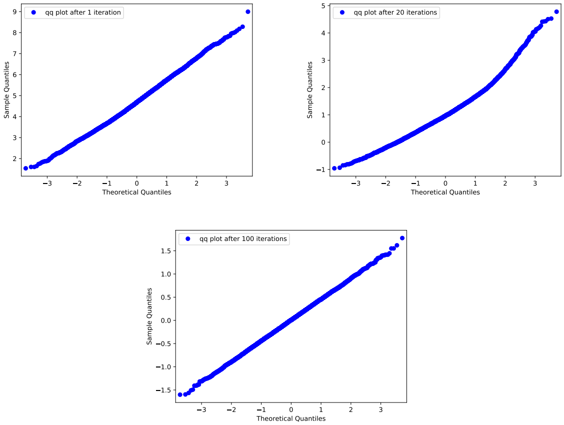
Verification: Gaussian shape



Probability density with gaussian fits.

- Starting with a gaussian initial distribution
- Strong deviation from the gaussian shape after 20 iterations
- Thermalisation: resume to gaussian shape after 100 iterations

Verification: Gaussian shape



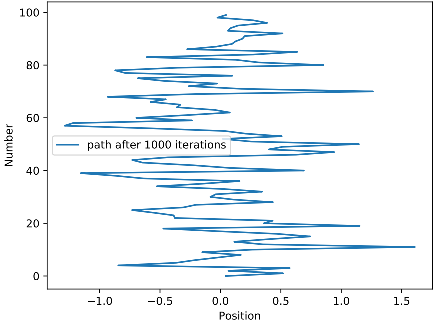
qq-plots: distribution after 1, 20 and 100 Metropolis iterations, compared with gaussian.

- Starting with a gaussian initial distribution
- Strong deviation from the gaussian shape after 20 iterations
- Thermalisation: resume to gaussian shape after 100 iterations

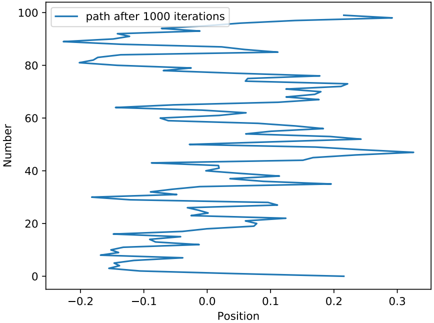
Verification: Results match the expectation

$\Rightarrow$ Code seems to be valid

Harmonic oscillator: Tracks



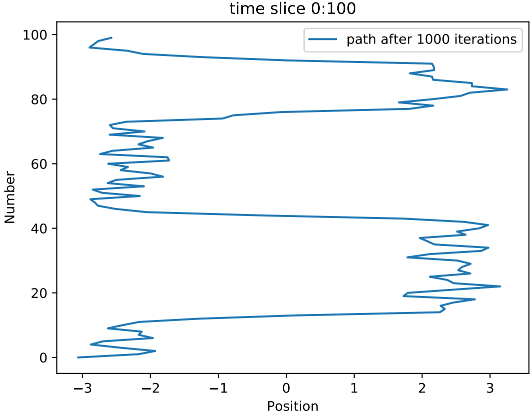
(a) $m = 0.25$



(b) $m = 10.0$

Typical tracks of the harmonic oscillator.

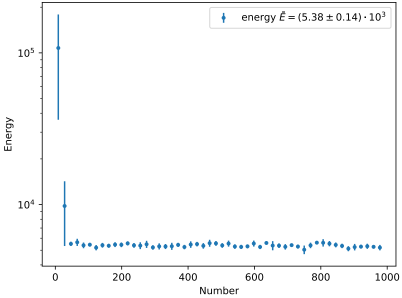
Harmonic oscillator: Tracks



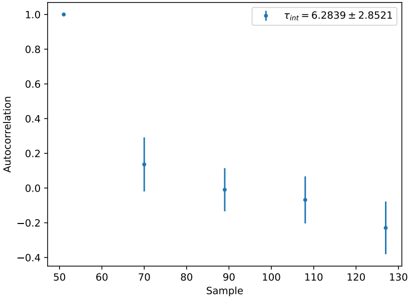
Typical track of the anharmonic oscillator.

- Transitions between minima (at ± 2.5) occur $\Rightarrow$ Tunnelling effect
- Transitions are very fast, as expected

Measurements: linear energy-$\hbar$-dependence



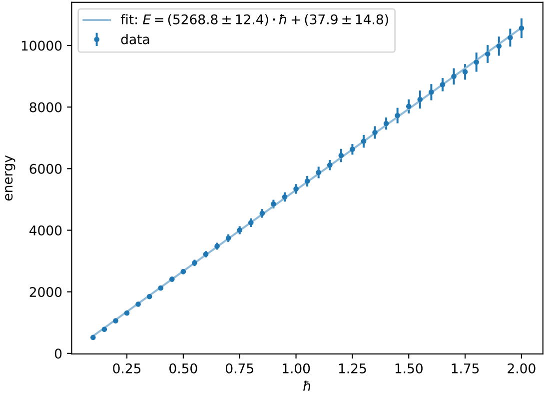
(a) Measurements



(b) Autocorrelation

- Thermalisation of energy occurs after 50 iterations.

Measurements: linear energy-$\hbar$-dependence



Classical limit energy, harmonic oscillator.

- Linear relation between E and $\hbar$ as expected from $E = \hbar\omega\left(\frac{1}{2} + n\right)$, for $n = 0$
- slope: $\frac{\omega}{2} = 5268.8(124)$

Measurements: tunnelling current

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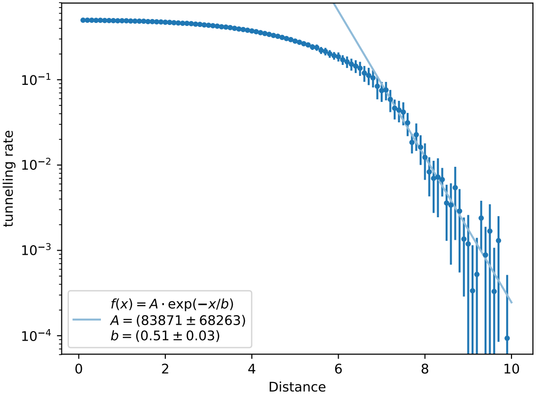
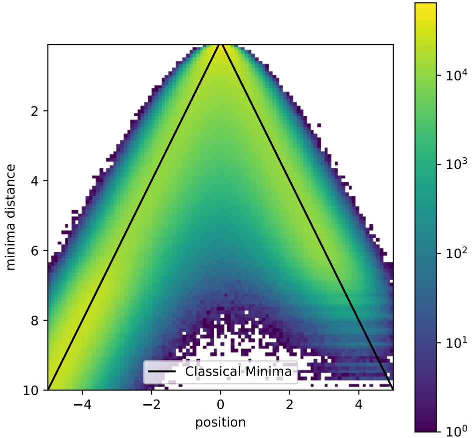


Tunnelling current depending on the distance of the classical minima.

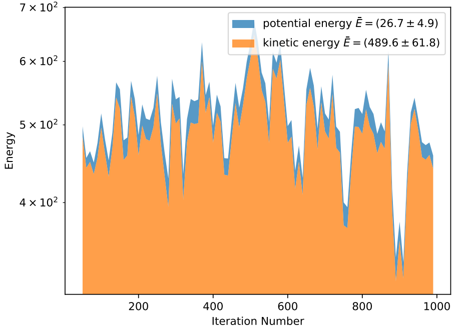
- Behaviour is different for distances $d > 7$ and $d < 7$
- Tunnelling current decays exponentially with increased distance of minima for $d > 7$.

Measurements: Probability distribution

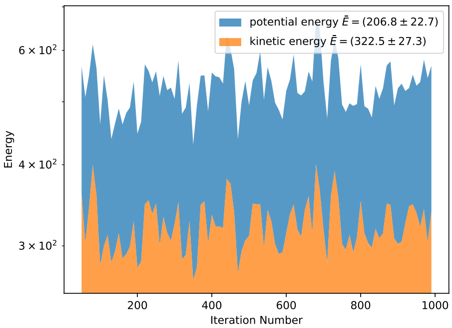


- Initially prepared in the left minimum
- Distributions are centred around the classical limits
- Tunnelling occurs rarely for large distances of minima

Measurements: Virial theorem



(a) Using $m = 10$.



(b) Using $m = 0.25$.

- Energy is not distributed evenly between kinetic and potential part
- Virial theorem does not hold for the produced data

Summary

- Classical limit confirmed validity of the code
- Metropolis-algorithm produces gaussian shaped distributions
- Linear relation between E and $\hbar$ could be confirmed
- Tunnelling current could be measured depending on the difference of the minima
- The Virial theorem does not apply for the simulated data

Thank you for your attention!

References

[1] C. M. Bender and T. T. Wu, *Anharmonic oscillator*, Phys. Rev. (2) **184**, 1231–1260 (1969).

[2] M. Rushka J. K. Freericks, *A Completely Algebraic Solution of the Simple Harmonic Oscillator*, arXiv:1912.08355 [quant-ph] (2019).

[3] M. Creutz and B. Freedman, *A statistical approach to quantum mechanics*, Annals of Physics, **132**, 427-462 (1981).

[4] R. Rodgers and L. Raes, *Monte Carlo simulations of harmonic and anharmonic oscillators in discrete Euclidean time*, DESY Summer Student Programme (2014).

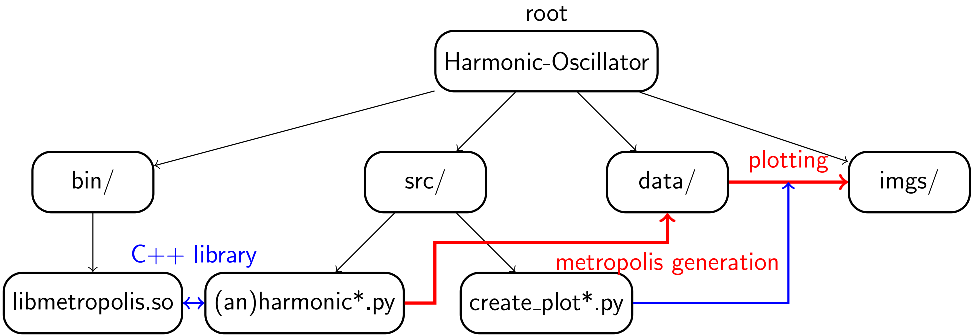
[5] G. C. Wick, *Properties of Bethe-Salpeter Wave Functions*, Physical Review. **96** 1124–1134 (1954).

[6] J. F. Cariñena, F. Falceto and M. F. Rañada, *A geometric approach to a generalized virial theorem*, arXiv:1209.4584 [math-ph] (2012).

[7] Public Github repository: Harmonic Oscillator, Benedikt Otto (s6beotto), `https://github.com/s6beotto/Harmonic-Oscillator`.

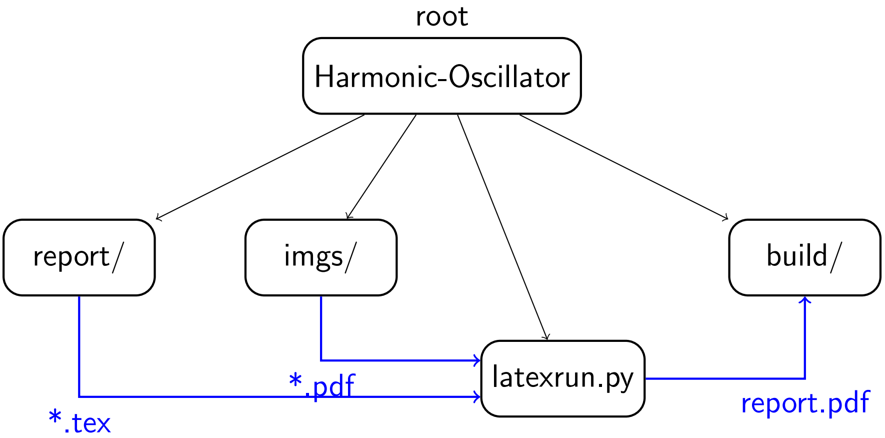
[8] Public Github repository: latexrun, Austin Clements (aclements), `https://github.com/aclements/latexrun`.

Data generation



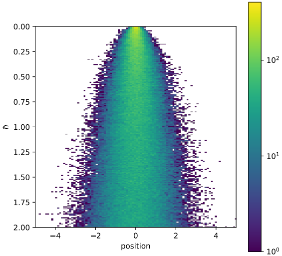
Directory structure of the project for data generation.

Report generation

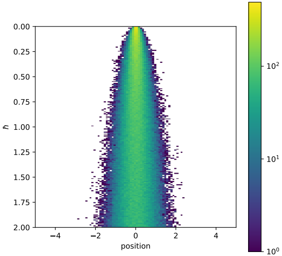


Directory structure of the project for report generation.

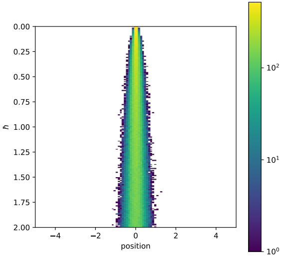
Harmonic oscillator: Tracks



(a) Using $m = 1$.



(b) Using $m = 10$.



(c) Using $m = 100$.

Classical limit of the harmonic oscillator for different masses.