Lattice theory and Metropolis simulation

Minuth, Maik
University of Dortmund

Fernández Caramés, Teresa
Universidad de Salamanca

This report contains a brief introduction to the lattice theory and path integral methods in Quantum Mechanics, including some short calculations on the harmonic oscillator. Numerical simulations based on the Metropolis algorithm have been performed to obtain some properties of the harmonic and anharmonic oscillator, such as the ground state energy, probability distribution and correlation function.

1 Introduction to Lattice Theory

1.1 Path Integrals

Since its introduction by Feynman (1948), the path integral method has become a very important tool for physicists. The Green Function for a quantum mechanical problem (so called Kernel) is calculated in this method by summing up all possible classical paths between two fixed points in space and time and weighting them with the factor $e^{\frac{i}{\hbar}S}$, where S is the classical action of the path[1]:

$$S = \int_{t_a}^{t_b} L(\dot{x}, x, t)dt \tag{1}$$

The path integral, which means integration over all possible paths, is formally written as:

$$K(b,a) = \int_a^b e^{iS[b,a]}\mathcal{D}x(t) \tag{2}$$

In order to illustrate how this is done, let's consider a particle moving in one dimension between $(x_a, 0)$ and (x_b, T). Because integration over a functional space has to be given a meaning, we wil introduce a time lattice to obtain a well defined expression. Therefore, the time axis is divided in $N+1$ steps of length $a = T/(N+1)$, so that every possible path on this time lattice is given by the set of coordinates $(x_1, x_2, \ldots, x_N)$. Each one of the x_j coordinates can vary from $-\infty$ to ∞. The action of the path will then be:

$$S_{lat}[x] = \sum_{j=1}^{N} a\left[\frac{M_0}{2}\frac{[x_{j+1}-x_j]^2}{a^2} - V(x_j)\right] \tag{3}$$

With this, the path integral takes on the form:

$$K(b,a)_{lat} = \int_{x_0=x_a}^{x_N=x_b} e^{iS_{lat}[x]} \prod_{j=1}^{N} \frac{dx_j}{A} \tag{4}$$

where A is a normalisation-factor.

The solution for the path integral in the continuum is obtained by taking the limit $N \to \infty$, therefore sending $a \to 0$, since the total time T is a fixed value.

1.2 Kernel for the Harmonic Oscillator

Here a short calculation is presented to show how the kernel of the harmonic oscillator can be obtained through the introduction of a time lattice.

The kernel we seek is given by:

$$K(b,a) = F(T)e^{G(x_a,x_b,T)} \tag{5}$$

$$F(T) = \left(\frac{m\omega}{2\pi i \sin\omega T}\right)^{1/2} \tag{6}$$

$$G(x_a,x_b,T) = \frac{im\omega}{2\sin\omega T}[(x_a^2+x_b^2)\cos\omega T - 2x_a x_b] \tag{7}$$

Our starting point will be equation (2) for the kernel.

[1] For convenience, from now on we set $\hbar = 1$

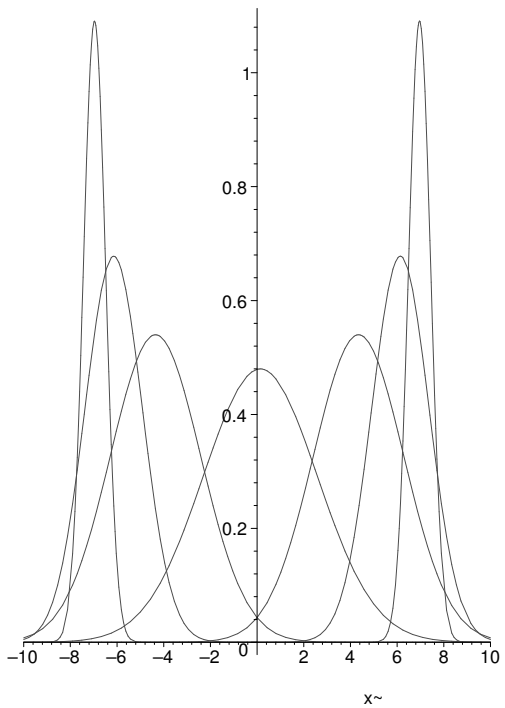

Fig. 1: *Time-developement of a non-centered Gaussian in the potential of a harmonic oscillator*

If $\bar{x}$ is the classical path minimizing the action, every path connecting points a and b can be written as: $x(t) = \bar{x}(t) + y(t)$, with $y(0) = y(T) = 0$. After some short calculations, we come to the following expression:

$$K(b,a) = F(T)e^{iS_{cl}[b,a]} \tag{8}$$

where

$$F(T) = \int_{y(0)=0}^{y(T)=0} e^{\frac{iM_0}{2a}(\frac{y^2}{a} - a\omega^2 y^2)} \mathcal{D}y(t) \tag{9}$$

and the second factor, the one that refers to the classical action, leads to the second factor in equation [5]. Therefore, our task now is to demonstrate that $F(T)$ gives the right dependency in ωT, according to eq. [6].

$$\int_{-\infty}^{\infty} e^{\frac{iM_0}{2a}\sum_{j=1}^{N}\left[\frac{[y_{j+1}-y_j]^2}{a} - a\omega^2 y_j^2\right]} \prod_{j=1}^{N} \frac{dy_j}{A} \tag{10}$$

We perform the following Fourier transformation, which will ease the calculations:

$$y_j = \sum_{p=1}^{N} b_p e^{i\omega_p j a} \tag{11}$$

$$\omega_p = \frac{p\pi}{(N+1)a} \tag{12}$$

This leads to the expresion below, where the integrand is diagonal in the new coordinates.

$$F(T) = J \int e^{\frac{iM_0}{2a}\sum\left(4\sin^2\frac{\omega_p a}{2} - a^2\omega^2\right)b_p^2} \prod_{j=1}^{N} db_j \tag{13}$$

Here, J is the Jacobian for the Fourier transformation independent of ω. Performing the integrations over these gaussian integrals, we arrive at:

$$F(T) = \left(\frac{2\pi a}{im}\right)^{N/2} J \prod_{p=1}^{N} \left(4\sin^2\frac{\omega_p a}{2} - a^2\omega^2\right)^{-1/2} \tag{14}$$

This product can be divided into two parts, one of them does not depend on ω, and therefore we store it with every other factor, that is independent of ω, in a constant factor $\mathcal{C}$.

$$F(T) = \mathcal{C}\left[\prod_{p=1}^{N}\left(1 - \frac{a^2(N+1)^2\omega^2}{j^2\pi^2}\right)\right]^{-1/2} \tag{15}$$

Performing the continuum limit ($a \to 0$,$N \to \infty$, $(N+1)a = T$), we finally get the desired dependency on ωT:

$$F(T) = \mathcal{C}\left(\frac{\omega T}{\sin\omega T}\right)^{1/2} \tag{16}$$

The constant factor $\mathcal{C}$ can as well be calculated by other means, like the comparison with the free particle kernel, to be:

$$\mathcal{C} = \sqrt{\frac{m}{2\pi i T}} \tag{17}$$

The Kernel can be used to calculate the time-developement of a given wave function $\psi(x)$ by:

$$\psi(x,T) = \int K(x,x',T)\psi(x')dx' \tag{18}$$

In figure 1, the form of a gaussian in a harmonic oscillator potential moving from right to left is shown (obtained by using Maple 8).

1.3 Statistical Approach

By making a transition to imaginary time $t \to i\tau$, therefore performing a rotation for the time-axis in the complex plane of $\pi/2$ (this is equivalent to the transition $a \to ia$ on the lattice), the Kernel changes to the following form:

$$K'(b,a)_{lat} = \int e^{-S'_{lat}[x]/\hbar} \prod_{j=1}^{N} \frac{dx_j}{A} \qquad (19)$$

with:

$$S'_{lat}[x] = \sum_{j=1}^{N} a \left[\frac{M_0}{2} \frac{[x_{j+1} - x_j]^2}{a^2} + V(x_j) \right] \qquad (20)$$

The Kernel now is identical to the partition function in statistical mechanics, and therefore we can apply the well-known numerical methods used there for our quantum mechanical problem. The Boltzmann factor is in this case $e^{-S'/\hbar}$, where $\hbar$ is equivalent to the temperature. So the path integral formulation of quantum mechanics provides us with a possibility to solve problems non-perturbatively.

The task now is to generate a great amount of paths distributed according to the Boltzmann factor, so called Heat Bath distribution, and use them to measure interesting observables.

2 Numerical Simulations

The problem studied by numerical implementation of this theory is that of the one dimensional oscillator, given by the following potential:

$$V(x) = \frac{1}{2}\mu^2 x^2 + \lambda x^4 \qquad (21)$$

2.1 Metropolis Algorithm

One of the easiest ways to implement the distribution of the Heat Bath situation in a numerical simulation is the algorithm introduced by N. Metropolis *et al.*. It starts with a certain path configuration, with N time slices, and changes the points of it one by one. The method of Metropolis begins by choosing randomly a new value x' with uniform probability. If the action is lowered by the replacement of x with x', the variable is set to this new value. If the action is increased, then a random number r with uniform distribution between 0 and 1 is generated, and the variable is changed by x' only if $e^{-\Delta S}$ is greater than r. Otherwise the lattice variable retains its previous value x. In this way, a second configuration is obtained.

By repeating this algorithm several times, an amount of paths is generated. They are distributed according to the Heat Bath situation.

The starting path is either a straight line or a completely random distribution of points on the time lattice between the selected start and end points. Those possibilities are called, respectively, cold and hot start. This is then thermalized by repeatedly performing the Metropolis algorithm for a certain amount of times. Once the path is already thermalized, we start storing generated paths for later evaluation. Between two consecutive stored paths, some more iterations are done in order to decorrelate the paths as much as possible.

2.2 Evaluation of the paths

2.2.1 Probability distribution

Once all the paths are stored, we want to know the probability for finding the particle in the interval $[x, x + \Delta x]$. In order to do so, the x-axis is divided into several intervals, so called bins, of width Δx. The computer counts the number of points in each one of these bins. Finally, the normalization is achieved by dividing these numbers by the total amount of points generated during the Metropolis process. In figure 2 and 3 the results for the harmonic[2], and anharmonic[3] oscillator are shown.

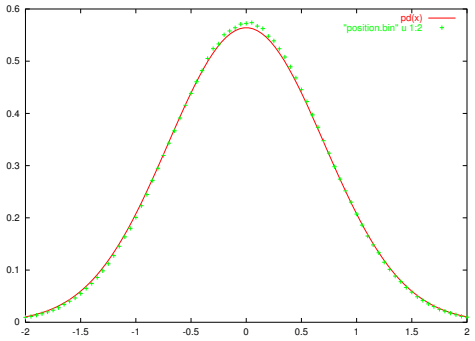

Fig. 2: *Ground state probability distribution for the harmonic oscillator (data and theoretical curve)*

[2] $(M_0 = 1, \mu^2 = 1, \lambda = 0)$
[3] $(M_0 = 1, \mu^2 = -4, \lambda = 1)$

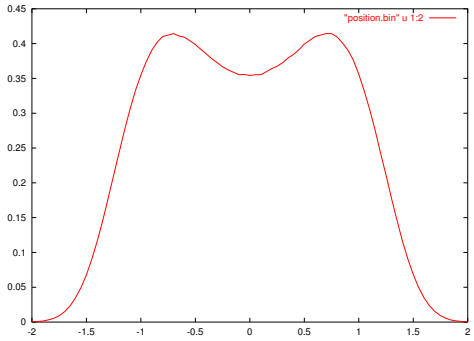

Fig. 3: *Ground state probability distribution for an anharmonic oscillator (interpolated data)*

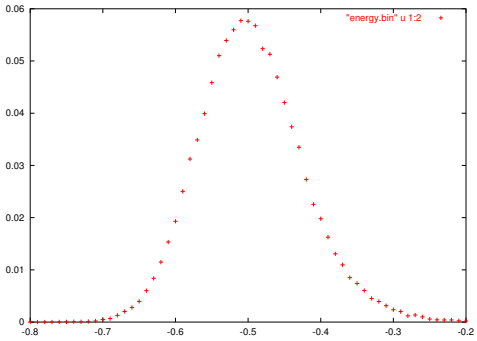

Fig. 5: *Energy distribution for an anharmonic oscillator*

2.2.2 Energy distribution

For every path, the average potential energy is calculated as:

$$\overline{E_{pot}}[x] = \frac{1}{N}\sum_{j=1}^{N} V(x_j) \tag{22}$$

In order to obtain the energy distribution, we use the same routine introduced for the probability distribution on the energy values. The results for the harmonic[4] and anharmonic oscillator[5] are shown in figure 4 and 5.

The potential energy distribution for the harmonic oscillator is centered near the theoretical value given by the well-known quantum mechanics expression for the ground-state $E_{0_{pot}} = \hbar\omega/4$ (with our parameters $E_{0_{pot}} = 0.25$).

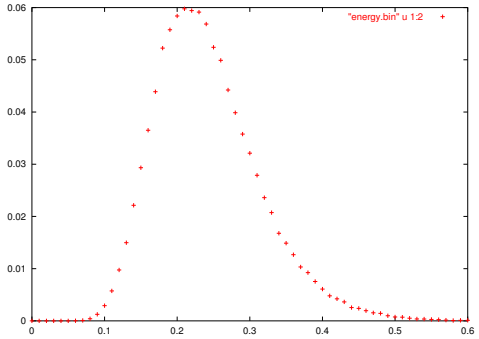

Fig. 4: *Energy distribution for the harmonic oscillator*

2.2.3 Correlation

Time correlation is obtained by taking the product of the position of two points in the same path separated by a time interval t, and averaging this product over all points and paths. This process has been done for different time intervals and plotted against the time in figure 6. Because of the logarithmic scale, it is easy to notice that the function is described by an exponential decay. The intercept of this is given by the expectation value of x^2, while the slope depends on the ground-state energy.

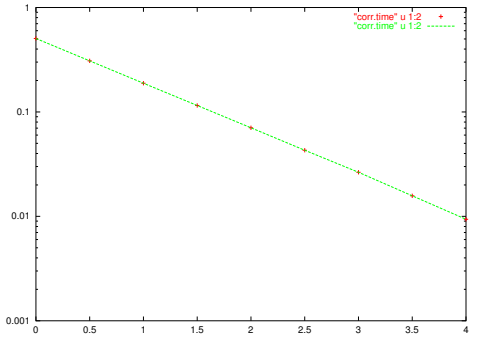

Fig. 6: *Correlation $\langle x(0)x(t)\rangle$ vs. t (data and interpolation)*

2.3 Lattice correction

The expectation value for x^2 is a function of the lattice constant, and theoretically, for the harmonic oscillator, given by the expression:

$$\langle x^2\rangle = \frac{1}{2\mu\sqrt{1+a^2\mu^2/4}} \cdot \frac{1+R^{T/a}}{1-R^{T/a}} \tag{23}$$

with:

$$R = 1 + \frac{a^2\mu^2}{2} - a\mu\sqrt{1+\frac{a^2\mu^2}{4}} \tag{24}$$

[4] $(M_0 = 1, \mu^2 = 1, \lambda = 0)$
[5] $(M_0 = 1, \mu^2 = -4, \lambda = 1)$

In order to test the simulation, the average of x^2 was calculated for several lattice constants and then plotted together with the theoretical curve against the lattice spacing(figure 7). The agreement between the generated values and the theoretical curve increased with the amount of evaluated points.

For the good agreement in our plot, the amount of evaluated points was in the order of 10^6, by setting a total time of $T = 500$.

It is easy to see that for small lattice spacings the theoretical value for the continuum (0.5 in this case) is approached, as a working lattice formulation requires.

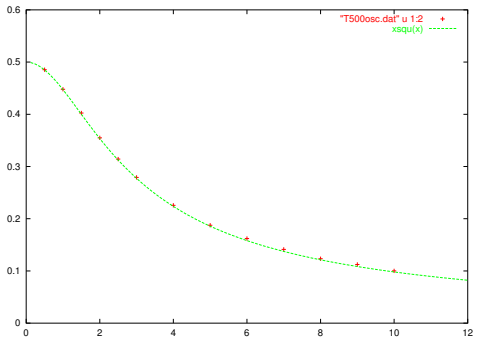

Fig. 7: $\langle x^2 \rangle$ *vs. a (data and theoretical curve)*

Acknowledgments

We want to thank Stephan Dürr for his kind help on the numerics and programming, Karl Jansen for his guidance and encouragement and in general all the members of the NIC group.

References

[1] R.P. Feynman and A.R.Hibbs, *Quantum Mechanics and Path Integrals*, (McGraw-Hill).

[2] M. Creutz and B. Freedman, *A Statistical Approach to Quantum Mechanics, Annals of Physics* **132**, 427-462 (1980).

[3] Heinz J. Rothe, *Lattice Gauge Theories - an Introduction* (World Scientific) .

[4] D. Verstegen, *Phys. Lett.* B **122**, 1 (1982).