Selected topics of lattice gauge theory

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1. Monte Carlo simulation of the harmonic oscillator

In this task we use the Metropolis algorithm to simulate the quantum mechanical harmonic oscillator and determine its ground state wave function numerically. The euclidean action of the harmonic oscillator with mass m, potential $V(X) = \frac{1}{2}kX^2$, and with periodic boundary conditions in τ is

$$S_E(\vec{X}) = \sum_{l=1}^{N} \frac{1}{2}\frac{m}{\Delta\tau}(X_{l+1} - X_l)^2 + \frac{1}{2}k\Delta\tau X_l^2. \tag{1}$$

The periodic boundary conditions imply the identification $X_{N+1} = X_1$.

a) Show that the euclidean action can be written as

$$S_E(\vec{x}) = \sum_{l=1}^{N} \hat{\omega}^{-1}(x_{l+1} - x_l)^2 + \hat{\omega}x_l^2 \tag{2}$$

where $\omega = \sqrt{\frac{k}{m}}$, $\hat{\omega} = \omega\Delta\tau$ and $\vec{x} = \sqrt{\frac{m\omega}{2}}\vec{X}$.

b) Write a program that uses the Metropolis algorithm to generate configurations $\vec{x}^{(m)}$ of the form

$$\vec{x}^{(m)} = (x_1^{(m)}, x_2^{(m)}, \ldots, x_N^{(m)}) \tag{3}$$

according to the distribution with the probability density

$$P(\vec{x}) = \frac{\exp(-S_E(\vec{x}))}{\int \cdots \int \mathrm{d}x_1 \ldots \mathrm{d}x_N \exp(-S_E(\vec{x}))}. \tag{4}$$

Here, the index (m) counts the different configurations generated by the Metropolis algorithm.

c) Use your program to simulate the harmonic oscillator. Use e.g. $N = 20$, $\hat{\omega} = 0.2$ for a start. Record the values of S_E and x_k during the simulation. Determine at which time S_E has started to fluctuate around its equilibrium value.

d) Determine numerically the probability density function to find the oscillator at x. Compare your result with the analytic function $|\psi_0(x)|^2$ known from quantum mechanics.

Hint: *You can calculate the probability density function by taking the histogram of the x_k^m values of your simulation. Make sure that you discard the first configurations of your simulation.*