Lattice Gauge Theory - Fall 2017 ETH Zürich

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Exercise Nr. 2

Discussion on October 3, 14:45

1) Properties of the Metropolis Algorithm

Consider the problem of computing the expectation value of an observable $\mathcal{O}$ with respect to a partition function $Z_f = \int\limits_{\infty}^{\infty} \mathrm{d}x\, f(x)$, i.e.:

$$< \mathcal{O} > = \frac{\int\limits_{\infty}^{\infty} \mathrm{d}x\, \mathcal{O}(x)\, f(x)}{\int\limits_{\infty}^{\infty} \mathrm{d}x\, f(x)}.$$

We will use this very simple problem to demonstrate how the Metropolis Algorithm works.
To do so we subdivide the x-axis into intervals $\Delta x_i = [x_i - \Delta/2, x_i + \Delta/2)$, $x_{i+1} = x_i + \Delta \forall i$. Now assume, we have a particle hopping around between neighboring x_i and that $\tilde{f}(x_i) = \frac{f(x_i)}{\sum\limits_i \Delta x_i f(x_i)}$ describes the probability to find it at position x_i. This means, that if you observe the particle for a long time t^{obs}, you should find that it has spent a time $t^{obs} \cdot \tilde{f}(x_i)$ at site x_i. Allowing the particle to attemp a hop only after discrete time steps, the number of time steps the particle has spent at at a site x_i divided by the total number of time steps for which we have observed the particle, should therefore approximate $f(x_i)$, and the approximation becomes better, the longer we observe the particle. This is in principle the way a Monte Carlo simulation works, where t^{obs} becomes the total Monte Carlo time, i.e. the length of the Markov chain and the time intervals correspond to its single elements.

1. Write down the balance equation which expresses that, as the particle must be around all the time somewhere in the system, the total probability to leave a site x_i must be the same as the total probability to enter this same site. Note that in order to be able to leave a site x_i the particle must first be located at this site. Call $p^{\pm}(x_i)$ the (yet unknown) pure transition probabilities to leave x_i in the positive/negative x-direction, provided the particle is already located at x_i.

2. Show that detailed balance
$$p^{\pm}(x_i)\tilde{f}(x_i) = p^{\mp}(x_{i\pm1})\tilde{f}(x_{i\pm1})$$
is a possibility to satisfy the balance equation from the previous task.

3. Prove that the *Metropolis rule*
   - always accept if $\tilde{f}(x') > \tilde{f}(x_i)$
   - accept with probability $p = \tilde{f}(x')/\tilde{f}(x_i)$ if $\tilde{f}(x') < \tilde{f}(x_i)$

   satisfies the detailed balance condition, where $x' \in \{x_{i+1}, x_{i-1}\}$ is the candidate for the location at which the particle could spend the next Monte Carlo time-interval if it does not remain at x_i.

4. What is the qualitative difference between the simple problem above, which could be easily solved in a simpler way, and the Ising model?

2) Metropolis Algorithm for Quantum Mechanics

Implement the Metropolis algorithm for the quantum mechanical system on a time crystal consisting of N time slices, based on the path integral given in the lecture and explained in detail on p. 440ff. in the paper of Creutz and Freedman [CF]. The discretized action is

$$S = a \sum_{i}^{N} \left(\frac{1}{2} m_0 \frac{(x_{i+1} - x_i)^2}{a^2} + V(x) \right), \qquad V(x) = \frac{1}{2}\mu^2 x^2 + \lambda x^4, \qquad x_0 = x_N$$

Draw the new x' from the uniform interval $[x - \Delta, x + \Delta]$ with $\Delta = 2\sqrt{a}$ and use the value $a = 0.1$, $\bar{n} = 10$ (number of Metropolis hits per site, Eq. 3.29 in [CF]).

For $m_0 = 1$ and the harmonic oscillator choice $\mu = 1$, $\lambda = 0$, perform simulations with various values of time slices N and analyze the continuum limit:

1. Generate a histogram for $|\psi_0(x)|^2$ by dividing the x-axis into bins of size Δx appropriately.
2. Determine the coefficients a,b for the probability distribution of locating the particle in the ground state at position x
$$|\psi_0(x)|^2 = a \exp(-bx^2)$$
for various N and compare your finding with the analytic result in App. C of [CF].

For $m_0 = 1$, and the anharmonic oscillator choice $\lambda = 1$, perform simulations with various (in particular also negative) values of μ^2:

1. Generate a histogram for $|\psi_0(x)|^2$ for each value of μ^2.
2. For $\mu^2 = -3$, measure the correlation function $\langle x(0)x(\tau)\rangle$ as a function of $0 \le \tau \le aN/2$ and extract from it the first two energy levels for various values of N.

Richard P. Feynman
(May 11, 1918 - February 15, 1988) was an American physicist.

[...] Feynman received a bachelor's degree from the Massachusetts Institute of Technology in 1939, and was named Putnam Fellow that same year. He received a Ph.D. from Princeton University in 1942, and in his theses applied the principle of stationery action to problems of quantum mechanics, laying the groundwork for the "path integral" approach and Feynman diagrams.

While researching his Ph.D., Feynman married his first wife and longtime sweetheart, Arline Greenbaum, who was already quite ill with tuberculosis. At Princeton, Robert W. Wilson encouraged Feynman to participate in the Manhattan Project. He did so, visiting his wife in a sanitarium in Albuquerque on weekends until her death in July 1945. He then immersed himself in work on the project and was present at the Trinity bomb test.

Hans Bethe made the 24 year old Feynman a group leader in the theoretical division. Although his work on the project was relatively removed from the major action, Feynman did calculate neutron equations for the Los Alamos "Water Boiler", a small nuclear reactor at the desert lab, in order to measure how close a particular assembly of fissile material was to becoming critical. After this work, he was transferred to the Oak Ridge facility, where he aided engineers in calculating safety procedures for material storage so that inadvertent criticality accidents could be avoided.

After the project, Feynman started working as a professor at Cornell University, and then moved to Cal Tech in Pasadena, Calif., where he did much of his best work including research in quantum electrodynamics, the physics of the superfluidity of supercooled liquid helium, and a model of weak decay. Feynman's collaboration on the latter with Murray Gell-Mann was seen as seminal, as the weak interaction was neatly described. He also developed Feynman diagrams, a bookkeeping device that helps in conceptualizing and calculating interactions between particles in spacetime, notably the interactions between electrons and their antimatter counterparts, positrons.

He later married Gweneth Howarth and had a son, Carl Richard, and a daughter, Michelle Catherine. In 1965, Feynman, along with Julian Schwinger and Shinichiro Tomonaga, shared the Nobel Prize in Physics for work in quantum electrodynamics. Feynman's popular lection series was published in "The Feynman Lectures", while his personal side was captured in "Surely You're Joking, Mr. Feynman!" and "What Do You Care What Other People Think?"

Feynman is also known for his work on the Space Shuttle Challenger accident investigation, shocking the world by demonstrating the failure of the O-Rings. He died February 15, 1988, at the age of 69, from several rare forms of cancer.

`[from http://www.atomicarchive.com/Bios/Feynman.shtml]`