Monte Carlo by Yuanda Liao

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This article is a note of Yuanda Liao's speech on Prof. Yang Qi's group meeting on October 16. 2021.

- Basic principles of Monte Carlo simulations.
- Metropolis algorithm.
- Wolff algorithm and why it works; some details about how to expand a cluster.
- Discrete path integral of quantum Ising models.

1 Cluster Update Algorithms

Monte Carlo algorithms in physics are usually performed by *importance sampling* and *Markov chain*, i.e. we construct a Markov chain of which the stable probability of a configuration is

$$p(C) = \frac{1}{Z} \mathrm{e}^{-F(C)}. \tag{1}$$

The Markov chain should be ergodic, and detailed balance condition

$$p(C) p(C \to C') = p(C') p(C' \to C). \tag{2}$$

Algorithm 1: Wolff update for classical Ising model

```
function kssolve(i) /* comment of functions                  */
    if Condition
        Then
    else
        else
    end
    for for condition /* for condition comment               */
        Do sth                                      /* asdf */
    end
    while the condition
        do something
        i = i + 1
    end
    return return value
    begin
        Mad
    end
end
```

2 Discrete Path Integral of Quantum Ising Models

The **transverse field Ising model** is defined as

$$H = -J \sum_{\langle i,j \rangle} \sigma_i^z \sigma_j^z - h \sum_i \sigma_i^x. \tag{3}$$

The (discrete) path integral in the σ^z basis is

$$
\begin{aligned}
Z &= \operatorname{tr} \mathrm{e}^{-\beta H} \\
&= \sum_{\tau} \mathrm{e}^{\Delta\tau J \sum_{i,j} \sigma_i^z(\tau)\sigma_j^z(\tau)} \langle \sigma^z(\tau+\Delta\tau) | \mathrm{e}^{\Delta\tau h \sum_i \sigma_i^x} | \sigma^z(\tau) \rangle
\end{aligned} \tag{4}
$$

With an error introduced by Trotter decomposition, we rephrase a problem in terms of operators into a problem in terms of path integral which only involves plus and multiplication of only ordinary numbers.

The temperature is introduced by the finite system effects in the temporal dimension. We usually fix $\Delta\tau$ and change the imaginary time steps, for several reasons:

- The Trotter error depends on $\Delta\tau$. Changing $\Delta\tau$ during calculation means the Trotter error differs significantly at different choices of (h, J). It is therefore very hard to systematically analyze the error.

- In finite size scaling, we should scale *both* space and time, so changing the number of imaginary time steps is not correct if we want to do finite size scaling.