# Computational Physics (Physics 760) Exercise #7

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## Tutorial Preparation

Download the Jupyter-Notebook **Exercise7.ipynb**.

- Download the files to your computer
- You can use `https://jupyter-jsc.fz-juelich.de/` if you do not have access to jupyter
- Start your JupyterLab on the LoginNode

  You should see your folder structure of `$Home` on the left site
- Drag and drop to copy the files to Jureca

The Jupyter-Notebook is meant to guide you through this exercise. It contains the (following) exercise, but also definitions and some more explanations.

## Tutorial Exercises

This weeks exercises introduces the Hybrid Monte Carlo algorithm at the example of the two dimensional $U(1)$ pure gauge theory, the gauge part in the Schwinger Model (more next week). Thus it suffices to introduce the concept of the HMC without introducing the fermions first, and hence without thinking too much about computational complexity.

**1: The Wilson Gauge Action**
The continuum action is

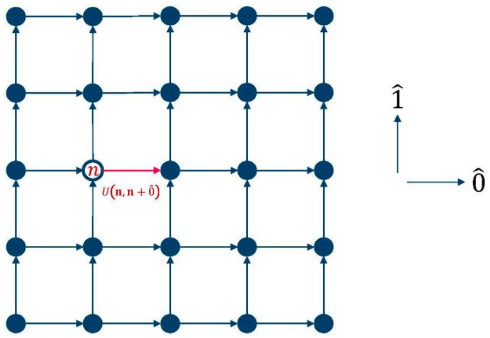
$$\begin{aligned} S\left(\Psi, \Psi^\dagger, A\right) &= \frac{2}{g^2} \int \Psi^\dagger(\mathbf{x}) \left(i\sigma^\mu D_\mu(\mathbf{x}) - m\right) \Psi(\mathbf{x}) + F^{\mu\nu}(\mathbf{x}) F_{\mu\nu}(\mathbf{x})\ d^2\mathbf{x} \\ &= S_F\left(\Psi, \Psi^\dagger, A\right) + S_G(A) \end{aligned} \tag{1}$$

where $\mathbf{x} = (t, x)$ denotes the 2 vector with one temporal $(t)$ and one spatial $(x)$ direction (1+1 dimensional), $\Psi(\mathbf{x})$ describes a two component spinor and $A_\mu(\mathbf{x}) \in \mathfrak{u}(1)$ represents the photon (scalar) field. Furthermore, $D_\mu(\mathbf{x}) = \partial_\mu - iA_\mu(\mathbf{x})$ is the Dirac operator and $F_{\mu\nu}(\mathbf{x}) = \partial_\mu A_\nu(\mathbf{x}) - \partial_\nu A_\mu(\mathbf{x})$ is the photon field strength tensor. Moreover, $\sigma_\mu$ are the Pauli matrices. This action can be identified as a two dimensional QED.
We will consider a lattice discretized theory. The fermion fields live on the sites of the lattice, the gauge fields live on the links. This week we only consider the pure gauge part to understand how an HMC algorithm can be implemented. For that, we introduce so-called "link variables" $U_\mu(\mathbf{n}) = e^{\mathrm{i}aA_\mu(a\mathbf{n})} \in U(1)$, hence the $U$ are just complex phases. Note that the link $U_\mu(n) = U(n, n+\hat{\mu})$ connects the sites $n$ and $n+\hat{\mu}$, where $\hat{\mu}$ is a unit step on the lattice in $\mu$ direction. The gauge action can now be defined using the plaquette:

$$S_A = -\beta \sum_{\mathbf{n}\in\Lambda} \Re\left(1 - P[U]_{\mu_x\mu_t}(\mathbf{n})\right)$$

$$\begin{aligned} P[U] = {} & U(\mathbf{n}, \mathbf{n}+\hat{0}) \\ & \cdot U(\mathbf{n}+\hat{0}, \mathbf{n}+\hat{0}+\hat{1}) \\ & \cdot U(\mathbf{n}+\hat{0}+\hat{1}, \mathbf{n}+\hat{1}) \\ & \cdot U(\mathbf{n}+\hat{1}, \mathbf{n}) \end{aligned}$$

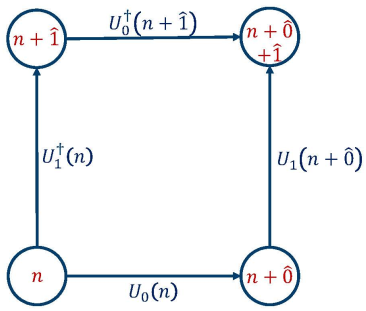
$$U(\mathbf{n}, \mathbf{n}+\hat{\mu}) = \exp iaA_\mu$$




Now, we can write (the reason does not matter here) $U(n, n-\hat{\mu}) = U^\dagger(n-\hat{\mu}, n)$, i.e. we can flip the direction, if we take the adjoint link. Similarly $U_{-\mu}(n+\hat{\mu}) = U_\mu^\dagger(n)$.

$$P[U] = U_0(n)U_1(n+\hat{0})U_0^\dagger(n+\hat{1})U_1^\dagger(n)$$


$$S_A = -\beta \sum_{n\in V} \Re(1 - P[U])$$




To summarize: we will only consider the (Wilson) gauge action (see $S_A$ above, modulo some factor). Implement the 2-dimensional Wilson gauge action, without using any explicit python loops.

a) Implement the plaquette.

$$P\left[U\right]_{\mu\nu}(\mathbf{n}) = U_\mu(\mathbf{n}) \cdot U_\nu(\mathbf{n}+\hat{\mu}) \cdot U_\mu^\dagger(\mathbf{n}+\hat{\nu}) \cdot U_\nu^\dagger(\mathbf{n})$$

b) Implement the Wilson gauge action.

$$S_G(U) = 2\beta \sum_{\mathbf{n}\in\Lambda} \mathrm{Re}\left(1 - P\left[U\right]_{\mu_t\mu_x}(\mathbf{n})\right)$$

**2: Change of Probability Distribution**

Show that

$$\langle O\rangle_\Phi = \frac{\int O[\Phi]\, e^{-S[\Phi]}\mathcal{D}[\Phi]}{\int e^{-S[\Phi]}\mathcal{D}[\Phi]} = \frac{\int O[\Phi]\, e^{-\mathcal{H}[\Phi,\pi]}\mathcal{D}[\Phi]\,\mathcal{D}[\pi]}{\int e^{-\mathcal{H}[\Phi,\pi]}\mathcal{D}[\Phi]\,\mathcal{D}[\pi]} = \langle O\rangle_{\Phi,\pi}$$

Hint:

- If you are not familiar handling path integrals, think about probability distributions.

**3: Force**

a) Show that the force is given by

$$F_\mu(\mathbf{n}) \equiv \frac{\partial \mathcal{H}(U,\pi)}{\partial U_\mu(\mathbf{n})} = -2\beta \,\mathrm{Im}\left[U_\mu(\mathbf{n}) K_\mu(\mathbf{n})\right] \tag{2}$$

where

$$K_\mu(\mathbf{n}) = U_\nu(\mathbf{n}+\hat{\mu}) \cdot U_\mu^\dagger(\mathbf{n}+\hat{\nu}) \cdot U_\nu^\dagger(\mathbf{n}) + U_\nu^\dagger(\mathbf{n}+\hat{\mu}-\hat{\nu}) \cdot U_\mu^\dagger(\mathbf{n}-\hat{\nu}) \cdot U_\nu(\mathbf{n}-\hat{\nu})\Big|_{\nu\neq\mu} \tag{3}$$

is the staple (implemented in Cell 7). Recall that the Hamiltonian is given with:

$$\mathcal{H}(U,\pi) = \frac{1}{2}\pi^2 + \beta \sum_{\mathbf{n}\in\Lambda} \mathrm{Re}\left(1 - P\left[U\right]_{\mu_x\mu_t}(\mathbf{n})\right) \tag{4}$$

b) What mathematical object is the force?

**4: Leapfrog within Gauge Group**
Recreate the leapfrog algorithm for the evolution of gauge fields. Steps that might help:

- Identify positions with gauge field ‘U = q‘.
- Identify momentum with momentum field ‘pi = p‘.
- Think about how gauge links can be updated to stay in the group.

**5: Leapfrog Algorithm Implementation**

a) Implement the Leapfrog algorithm.

b) Check Reversibility and Energy conservation.

c) Check correctness of HMC and by convexity that $\langle \delta H \rangle\rangle$ is non-negative in your simulation, exp, $1 = \langle \exp(-\delta H)\rangle \geq \exp\{-\langle \delta H \rangle\rangle\}$

**6: Hybrid Monte Carlo**
Implement the Hybrid Monte Carlo algorithm.