FT-HMC code for 2D $U(1)$

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Abstract

Brief description of the code. Many features mimic the qlat [1].

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Contents

1. Physical system

Path integral

$U(1)$ lattice gauge theory on T^2:

$$Z_{\beta,\theta} \equiv \int (dU)\, e^{-S(U)+i\theta Q(U)}, \tag{1.1}$$

where $U_{x,\mu}$ are $U(1)$-valued link variables:

$$U_{x,\mu} = e^{i\phi_{x,\mu}} \tag{1.2}$$

and (dU) the Haar measure:

$$(dU) = \prod_{x,\mu} \Big(\frac{d\phi_{x,\mu}}{2\pi} \Big). \tag{1.3}$$

We choose as $S(U)$ the Wilson action [2]:

$$S(U) \equiv -\beta \sum_x \cos \kappa_x \tag{1.4}$$

and $Q(U)$ the integer-valued topological charge [3, 4]:

$$Q(U) \equiv \frac{1}{2\pi} \sum_x \kappa_x, \tag{1.5}$$

where κ_x is the plaquette angle:

$$\begin{aligned} \kappa_x &\equiv \frac{1}{i} \ln \big(U_{x,0} U_{x+0,1} U^\dagger_{x+1,0} U^\dagger_{x,1} \big) \\ &= \phi_{x,0} + \phi_{x+0,1} - \phi_{x+1,0} - \phi_{x,1} \pmod{2\pi}, \end{aligned} \tag{1.6}$$

where it is assumed that we take the principal branch of the logarithm:

$$\kappa_x \in [-\pi, \pi). \tag{1.7}$$

Classically, the gauge potential $A_{x,\mu}$ in the continuum is defined as:

$$\phi_{x,\mu} = aA_{x,\mu}, \tag{1.8}$$

where a is the lattice spacing. By scaling β as:

$$\beta = \frac{1}{(ag)^2}, \tag{1.9}$$

we have

$$S(U) \sim \frac{a^2}{2g^2}\sum_x F_{01}^2 \sim \frac{1}{4g^2}\int d^2x\, F_{\mu\nu}^2 \tag{1.10}$$

and

$$Q(U) \sim \frac{1}{2\pi}a^2\sum_x F_{01} \sim \frac{1}{2\pi}\int d^2x\, F_{01}, \tag{1.11}$$

where

$$F_{\mu\nu} \equiv \partial_\mu A_\nu - \partial_\nu A_\mu. \tag{1.12}$$

<u>Exact solutions</u>

We compute the partition function:

$$Z_{\beta,\theta} = \int (dU)\prod_x e^{\beta\cos\kappa_x + \frac{i\theta}{2\pi}\kappa_x}. \tag{1.13}$$

We can use the Fourier expansion:

$$e^{\beta\cos\kappa + \frac{i\theta}{2\pi}\kappa} = \sum_{n\in\mathbb{Z}}\lambda_n(\beta,\theta)e^{in\kappa}, \tag{1.14}$$

where

$$\lambda_n(\beta,\theta) \equiv \int_{-\pi}^{\pi}\frac{d\kappa}{2\pi}\, e^{-i\nu\kappa}e^{\beta\cos\kappa}\Big|_{\nu=n-\theta/2\pi} \tag{1.15}$$

$$\sim \frac{e^\beta}{\sqrt{2\pi\beta}}\sum_{k\geq 0}(\nu,k)\left(\frac{-1}{2\beta}\right)^k\Big|_{\nu=n-\theta/2\pi} \tag{1.16}$$

with

$$(\nu,k) \equiv \frac{\Gamma(\nu+k+1/2)}{k!\,\Gamma(\nu-k+1/2)} = \frac{\{4\nu^2-1^2\}\{4\nu^2-3^2\}\cdots\{4\nu^2-(2k-1)^2\}}{2^{2k}\cdot k!}. \tag{1.17}$$

For $\theta = 0$, $\lambda_n(\beta,\theta)$ is identical to the modified Bessel function $I_\nu(\beta)$, but they are different generically.[1] We now have

$$Z_{\beta,\theta} = \int (dU)\prod_x\sum_{n_x}\lambda_{n_x}(\beta,\theta)e^{in_x\kappa_x} = \sum_n \lambda_n(\beta,\theta)^{\hat{V}}, \tag{1.18}$$

[1]The integral (1.15) is an even function of ν, but $I_\nu(\beta)$ is not.

where $\hat{V}$ is the lattice volume (in the lattice units).

We compute some expectation values for the case $\theta = 0$. The average plaquette can be calculated as

$$\begin{aligned}
\langle \cos \kappa_x \rangle &= \frac{1}{\hat{V}} \frac{d}{d\beta} \ln Z_{\beta,\theta=0} \\
&= \frac{\sum_n \left[(I_{n+1}(\beta) + I_{n-1}(\beta))/2 \right] \cdot I_n(\beta)^{\hat{V}-1}}{\sum_n I_n(\beta)^{\hat{V}}} \\
&\to \frac{I_1(\beta)}{I_0(\beta)} \sim \left(1 - \frac{1}{2\beta} \right) \quad (\beta \to \infty),
\end{aligned} \tag{1.19}$$

where we used that $(0,0) = (1,0) = 1$, $(0,1) = -1/4$ and $(1,1) = 3/4$. We define the average energy density by:

$$e \equiv \frac{1}{a^4 \hat{V}} \sum_x (1 - \cos \kappa_x) \to \frac{1}{2V} \int d^2x \, F_{01}^2 \quad (a \to 0), \tag{1.20}$$

where $V \equiv a^2 \hat{V}$ is the physical volume of the system. This is actually a divergent quantity as can be seen from that:

$$\langle e \rangle \sim \frac{g^2}{2a^2}. \tag{1.21}$$

The UV fluctuation is so strong that the energy is divergent. This is reflected to the fact that there is no correlation length in this system, which can be seen from the above calculation by modifying β to β_x and by taking the derivatives with respect to β_x:

$$\langle \cos^2 \kappa_x \rangle = \frac{\sum_n \left[(I_{n+2}(\beta) + I_n(\beta)) + I_{n-2}(\beta))/4 \right] \cdot I_n(\beta)^{\hat{V}-1}}{\sum_n I_n(\beta)^{\hat{V}}}, \tag{1.22}$$

$$\langle \cos \kappa_x \cos \kappa_y \rangle = \frac{\sum_n \left[(I_{n+1}(\beta) + I_{n-1}(\beta))^2/4 \right] \cdot I_n(\beta)^{\hat{V}-2}}{\sum_n I_n(\beta)^{\hat{V}}} \quad (x \neq y). \tag{1.23}$$

We also calculate the susceptibility:

$$\begin{aligned}
\chi_Q &\equiv \frac{1}{V} \langle Q^2 \rangle \\
&= -\frac{1}{V} \frac{d^2}{d\theta^2} \ln Z_{\beta,\theta} \Big|_{\theta=0} \\
&= -\frac{1}{V} \frac{1}{Z_{\beta,\theta}} \hat{V} \sum_n \lambda_n^{\hat{V}-1} \cdot \frac{d^2 \lambda_n}{d\theta^2} \Big|_{\theta=0} \\
&\sim -\frac{1}{a^2} \frac{1}{\lambda_0(\beta,\theta)} \frac{d^2 \lambda_0}{d\theta^2} \Big|_{\theta=0},
\end{aligned} \tag{1.24}$$

where we used the fact $(d\lambda_n/d\theta)|_{\theta=0} = 0$. To get the continuum limit, we take the derivative of eq. (1.16) with respect to ν. Using the polygamma function:

$$\psi^{(m)}(z) \equiv \frac{d^m}{dz^m} \ln \Gamma(z), \tag{1.25}$$

we have:

$$(2\pi)\frac{d}{d\theta}\lambda_n(\beta,\theta) \sim \frac{e^\beta}{\sqrt{2\pi\beta}}\sum_{k\geq 0}(\nu,k)A(\nu,k)\Big(\frac{-1}{2\beta}\Big)^k\Big|_{\nu=n-\theta/2\pi}, \tag{1.26}$$

$$(2\pi)^2\frac{d^2}{d\theta^2}\lambda_n(\beta,\theta) \sim \frac{e^\beta}{\sqrt{2\pi\beta}}\sum_{k\geq 0}(\nu,k)\big\{A(\nu,k)^2+B(\nu,k)\big\}\Big(\frac{-1}{2\beta}\Big)^k\Big|_{\nu=n-\theta/2\pi} \tag{1.27}$$

with

$$A(\nu,k) \equiv \psi^{(0)}(\nu+k+1/2)-\psi^{(0)}(\nu+k-1/2), \tag{1.28}$$

$$B(\nu,k) \equiv \psi^{(1)}(\nu+k+1/2)-\psi^{(1)}(\nu+k-1/2). \tag{1.29}$$

Therefore,

$$\begin{aligned}\chi_Q &\sim -\frac{1}{a^2}\frac{1}{I_0(\beta)}\frac{d^2\lambda_0}{d\theta^2}\Big|_{\theta=0}\\ &\sim -\frac{1}{a^2}\cdot 1\cdot\Big(\frac{-1}{4}\Big)\cdot(-8)\cdot\Big(\frac{-1}{2\beta}\Big) = g^2,\end{aligned} \tag{1.30}$$

where we used that $A(0,0)=A(0,1)=0$, $B(0,0)=0$ and $B(0,1)=-8$. The susceptibility has a finite value in the continuum limit.

2. Field-transformed HMC

The contents expressed here was first developed by [5] for $SU(3)$ on T^4.

Transformation

$$U_{x,\mu} \to U^{(\epsilon)}_{x,\mu} \equiv \mathcal{F}_\epsilon(U)_{x,\mu} \equiv e^{\epsilon\tilde{\partial}_{x,\mu}\tilde{S}(U)}U_{x,\mu}. \tag{2.1}$$

We choose the kernel $\tilde{S}(U)$ to be the plaquettes:

$$\tilde{S}(U) = \sum_x \cos\kappa_x. \tag{2.2}$$

We recursively define for $\ell \geq 1$:

$$S_{\ell\epsilon}(U) \equiv S_{(\ell-1)\epsilon}(\mathcal{F}_\epsilon(U)) - \ln\det\mathcal{F}_{\epsilon *}(U), \tag{2.3}$$

where $S_0(U)=S(U)$ and $\mathcal{F}_{\epsilon *}(U,\tilde{U})$ is the Jacobian of the transformation (2.1). By acting $d \equiv \sum_{x,\mu} d\theta_{x,\mu}\partial_{x,\mu}$ to eq. (2.1), we find

$$\mathcal{F}_{\epsilon *}(U)_{x,\mu|y,\nu} = \delta_{xy}\delta_{\mu\nu} + \epsilon\partial_{y,\nu}\partial_{x,\mu}\tilde{S}(U). \tag{2.4}$$

To the leading order in ϵ,

$$S_{\ell\epsilon}(U) = S_{(\ell-1)\epsilon}(U) + \epsilon \sum_{x,\mu} \partial_{x,\mu}\tilde{S}(U)\partial_{x,\mu}S(U) - \epsilon \sum_{x,\mu} \partial_{x,\mu}^2 \tilde{S}(U). \tag{2.5}$$

Explicitly,

$$S_{\ell\epsilon}(U) = S_{(\ell-1)\epsilon}(U) + \epsilon \sum_{x} \Big[4\beta \sin^2 \kappa_x - \beta \sum_{\mu=\pm 0,\pm 1} \sin \kappa_{x+\mu} \sin \kappa_x + 4 \cos \kappa_x \Big]. \tag{2.6}$$

Note that, from eq. (2.4),

$$\partial_{y,\nu} = \partial_{x,\mu}^{(\epsilon)} \mathcal{F}_{\epsilon *}(U)_{x,\mu|y,\nu}. \tag{2.7}$$

Therefore, from eq. (2.3),

$$\partial_{y,\nu}S_{\ell\epsilon}(U) = \sum_{x,\mu} \left[\delta_{xy}\delta_{\mu\nu} + \epsilon \partial_{y,\nu}\partial_{x,\mu}\tilde{S}(U)\right] \partial_{x,\mu}^{(\epsilon)} S_{(\ell-1)\epsilon}(U^{(\epsilon)}) - \mathrm{tr}\big[\mathcal{F}_{\epsilon *}(U)^{-1}\partial_{y,\nu}\mathcal{F}_{\epsilon *}(U)\big]. \tag{2.8}$$

In practice, we deal with finite ϵ. To ensure that the map is invertible, we perform the even/odd partitioning. In terms of the angle variables, the transformation can be rewritten as:

$$\theta_{x,\mu}^{(\epsilon)} = \theta_{x,\mu} - \epsilon(\sin \kappa_{x'} - \sin \kappa_{x''}), \tag{2.9}$$

where

$$x' = x,\ x'' = x - 1 \quad (\mu = 0) \tag{2.10}$$

$$x' = x - 0,\ x'' = x \quad (\mu = 1). \tag{2.11}$$

To invert eq. (2.9), we rewrite the equation as:

$$f(X) = Z_{x,\mu}(\theta)|_{\theta=\theta^{(\epsilon)}-\epsilon X}, \quad X = f(X), \tag{2.12}$$

where

$$Z_{x,\mu}(\theta) \equiv \partial_{x,\mu}\tilde{S}(U) = -\sin \kappa_{x'} + \sin \kappa_{x''}. \tag{2.13}$$

Then, for $\epsilon < 1/2$ the map f defines the contraction mapping because:

$$\begin{aligned} |f(X) - f(Y)| &= | - \sin(\varphi + \epsilon X) + \sin(\varphi' - \epsilon X) + \sin(\varphi + \epsilon Y) - \sin(\varphi' - \epsilon Y)| \\ &= \Big| - 2\cos\Big(\varphi + \frac{\epsilon}{2}(X-Y)\Big) \sin\Big(\frac{\epsilon}{2}(X-Y)\Big) \\ &\qquad + 2\cos\Big(\varphi' + \frac{\epsilon}{2}(X-Y)\Big) \sin\Big(\frac{\epsilon}{2}(X-Y)\Big)\Big| \end{aligned} \tag{2.14}$$

$$\leq 2\epsilon|X - Y|. \tag{2.15}$$

3. Code

The code consists of the `main.c` and the following header files:

util.h some utility functions (print functions for vectors, projection from $\mathbb{R}$ to $U(1)$).

lattice.h defines the `Lattice` class, which describes the geometry of the lattice.

coord.h defines the `Coord` class, which describes a point x on the lattice.

scalar_field.h defines the `ScalarField` class, which describes the field $\theta_{x,\mu}$ on the lattice. We use it for the angular variables.

action.h defines the `WilsonAction` class, which describes the action function S.

corr.h defines the `Corr` class, which gives the correlator functions $\cos\kappa_x \cdot \cos\kappa_y$.

rnd.h defines the `Rnd` class, which gives a set of mt19937 generators on each site or link.

hmc.h defines the `HMC` class, which gives the *ordinary* HMC algorithm.

kernel.h defines the `Kernel` class, which describes the kernel $\tilde{S}$ for the field transformations.

field_trsf.h defines the `FieldTrsf` class, which describes the infinitesimal map $\mathcal{F}_\epsilon$.

ft_hmc.h defines the `FT_HMC` class, which gives the FT-HMC algorithm.

The present code calculates and records the

- average plaquette
- two-point functions
- topological charge.

The plaquette and the topological charge are recorded for both the physical field U and the auxiliary field V.

The code is aimed to be run on laptops and uses `c++17` for `filesystem`. The remaining part only uses `c++11`. It can run with openmp. No MPI calls. It generates `500 configurations` with two-step Wilson-flowed HMC in $\sim$ `30 sec` for 8×8 lattice on my workstation (with OpenMP). It creates `./result/` directory, in which the observable data are stored, and a few log files. The contents written in this paragraph are mostly described in `main.c`.

One can compile and run the code with `make IS_FTHMC=0; make run`. The included `analysis.ipynb` can be used to analyze observable data. The exact solutions (or their approximated functions) are written here for the checks.

References

[1] L. Jin, "Qlattice," https://github.com/jinluchang/Qlattice

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[3] M. Luscher, "Topology of Lattice Gauge Fields," Commun. Math. Phys. **85**, 39 (1982) doi:10.1007/BF02029132

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[5] M. Luscher, "Trivializing maps, the Wilson flow and the HMC algorithm," Commun. Math. Phys. **293**, 899-919 (2010) doi:10.1007/s00220-009-0953-7 [arXiv:0907.5491 [hep-lat]].