1 Hamiltonian Monte Carlo for fuzzy spaces

1.1 Statement of the problem

The fuzzy space action considered here is:

$$S[D] = g_2 \operatorname{Tr} D^2 + \operatorname{Tr} D^4 \tag{1}$$

where $g_2 \in \mathbb{R}$ and D is of the form:

$$D = \sum_i \omega_i \otimes \left(M_i \otimes I + \epsilon_i I \otimes M_i^T \right) \tag{2}$$

for Hermitian ω_i and M_i, and $\epsilon_i = \pm 1$.
The dynamical variables in the Monte Carlo are the $n \times n$ matrices M_i. Hamiltonian Monte Carlo requires to take derivatives such as:

$$\frac{\partial S[M_i]}{\partial M_k} \tag{3}$$

which amounts to finding formulas for terms like:

$$\frac{\partial \operatorname{Tr} D^p}{\partial M_k}. \tag{4}$$

In the following, formulas for $p = 2$ and $p = 4$ are developed.

1.2 Matrix calculus

Let $A \in M_n(\mathbb{C})$ and $f(A)$ be a complex valued function of A. The derivative of f with respect to A is defined in components as the $n \times n$ matrix:

$$\left(\frac{\partial f}{\partial A} \right)_{lm} \equiv \frac{\partial f}{\partial A_{lm}}. \tag{5}$$

The two special cases of interest here are:

$$\frac{\partial \operatorname{Tr} A}{\partial A} = I \tag{6}$$

$$\frac{\partial \operatorname{Tr} AB}{\partial A} = B^T. \tag{7}$$

1.3 The case $p = 2$

When $p = 2$ the M_i matrices are decoupled:

$$\operatorname{Tr} D^2 = \sum_i \operatorname{Tr} \omega_i^2 (2n \operatorname{Tr} M_i^2 + 2\epsilon_i (\operatorname{Tr} M_i)^2). \tag{8}$$

Taking a derivative with respect to M_k yields:

$$\begin{aligned} \frac{\partial}{\partial M_k} \left(\sum_i \operatorname{Tr} \omega_i^2 (2n \operatorname{Tr} M_i^2 + 2\epsilon_i (\operatorname{Tr} M_i)^2) \right) &= \\ \sum_i \delta_{ik} \operatorname{Tr} \omega_i^2 \left(4n M_i^T + 4\epsilon_i (\operatorname{Tr} M_i) I \right) &= \\ 4C \left(n M_k^T + \epsilon_k (\operatorname{Tr} M_k) I \right) & \end{aligned} \tag{9}$$

where $C \equiv \operatorname{Tr} \omega_i^2$ is the dimension of the Clifford module.

1.4 The case $p = 4$

First expand $\operatorname{Tr} D^4$:

$$\begin{aligned} \operatorname{Tr} D^4 = \sum_{i_1, i_2, i_3, i_4} & \operatorname{Tr}(\omega_{i_1} \omega_{i_2} \omega_{i_3} \omega_{i_4}) \cdot \\ \Big(\; & n[1 + \epsilon_{i_1} \epsilon_{i_2} \epsilon_{i_3} \epsilon_{i_4} *] \operatorname{Tr}(M_{i_1} M_{i_2} M_{i_3} M_{i_4}) \;\; + \\ & \operatorname{Tr} M_{i_1} [\epsilon_{i_1} + \epsilon_{i_2} \epsilon_{i_3} \epsilon_{i_4} *] \operatorname{Tr}(M_{i_2} M_{i_3} M_{i_4}) \;\; + \\ & \operatorname{Tr} M_{i_2} [\epsilon_{i_2} + \epsilon_{i_1} \epsilon_{i_3} \epsilon_{i_4} *] \operatorname{Tr}(M_{i_1} M_{i_3} M_{i_4}) \;\; + \\ & \operatorname{Tr} M_{i_3} [\epsilon_{i_3} + \epsilon_{i_1} \epsilon_{i_2} \epsilon_{i_4} *] \operatorname{Tr}(M_{i_1} M_{i_2} M_{i_4}) \;\; + \\ & \operatorname{Tr} M_{i_4} [\epsilon_{i_4} + \epsilon_{i_1} \epsilon_{i_2} \epsilon_{i_3} *] \operatorname{Tr}(M_{i_1} M_{i_2} M_{i_3}) \;\; + \\ & [\epsilon_{i_1} \epsilon_{i_2} + \epsilon_{i_3} \epsilon_{i_4}] \operatorname{Tr}(M_{i_1} M_{i_2}) \operatorname{Tr}(M_{i_3} M_{i_4}) \;\; + \\ & [\epsilon_{i_1} \epsilon_{i_3} + \epsilon_{i_2} \epsilon_{i_4}] \operatorname{Tr}(M_{i_1} M_{i_3}) \operatorname{Tr}(M_{i_2} M_{i_4}) \;\; + \\ & [\epsilon_{i_1} \epsilon_{i_4} + \epsilon_{i_2} \epsilon_{i_3}] \operatorname{Tr}(M_{i_1} M_{i_4}) \operatorname{Tr}(M_{i_2} M_{i_3}) \; \Big) \end{aligned} \tag{10}$$

where $*$ denotes complex conjugation of everything that appears on the right, and the relation $M^T = M^*$ has been used. The reality of the expression comes from the fact that a simultaneous index exchange $i_1 \leftrightarrow i_4$ and $i_2 \leftrightarrow i_3$ is equivalent to taking the complex conjugate.

Taking a matrix derivative with respect to M_k results in non-vanishing contributions when $k = i_1, k = i_2, k = i_3$ or $k = i_4$:

$$\frac{\partial}{\partial M_k} \operatorname{Tr} D^4 = \sum_{i_1,i_2,i_3,i_4} \operatorname{Tr}(\omega_{i_1}\omega_{i_2}\omega_{i_3}\omega_{i_4}) \cdot \Big(\delta_{ki_1} A(i_1,i_2,i_3,i_4) + \delta_{ki_2} A(i_2,i_3,i_4,i_1) + \delta_{ki_3} A(i_3,i_4,i_1,i_2) + \delta_{ki_4} A(i_4,i_1,i_2,i_3)\Big) \tag{11}$$

where $A(a,b,c,d)$ is the following $n \times n$ matrix:

$$\begin{aligned} A(a,b,c,d) \equiv\ & n[\mathrm{T} + \epsilon_a\epsilon_b\epsilon_c\epsilon_d *] M_b M_c M_d + \\ & I[\epsilon_a + \epsilon_b\epsilon_c\epsilon_d *] \operatorname{Tr} M_b M_c M_d + \\ & \operatorname{Tr} M_b [\epsilon_b \mathrm{T} + \epsilon_a\epsilon_c\epsilon_d *] M_c M_d + \\ & \operatorname{Tr} M_c [\epsilon_c \mathrm{T} + \epsilon_a\epsilon_b\epsilon_d *] M_b M_d + \\ & \operatorname{Tr} M_d [\epsilon_d \mathrm{T} + \epsilon_a\epsilon_b\epsilon_c *] M_b M_c + \\ & M_b^T [\epsilon_a\epsilon_b + \epsilon_c\epsilon_d] \operatorname{Tr} M_c M_d + \\ & M_c^T [\epsilon_a\epsilon_c + \epsilon_b\epsilon_d] \operatorname{Tr} M_b M_d + \\ & M_d^T [\epsilon_a\epsilon_d + \epsilon_b\epsilon_c] \operatorname{Tr} M_b M_c \end{aligned} \tag{12}$$

with T denoting transposition of everything that appears on the right.
Now it is useful to write Eq.(11) symbolically as:

$$\frac{\partial}{\partial M_k} \operatorname{Tr} D^4 = \sum_{i_1,i_2,i_3,i_4} \mathcal{B}(i_1,i_2,i_3,i_4) \tag{13}$$

and notice that a simultaneous exchange of indices $i_1 \leftrightarrow i_4$ and $i_2 \leftrightarrow i_3$ is equivalent to taking the Hermitian conjugate:

$$\mathcal{B}(i_1,i_2,i_3,i_4)^\dagger = \mathcal{B}(i_4,i_3,i_2,i_1). \tag{14}$$

One can then introduce an equivalence relation $(i_1,i_2,i_3,i_4) \sim (i_4,i_3,i_2,i_1)$ and restrict the sum on the equivalence classes:

$$\frac{\partial}{\partial M_k} \operatorname{Tr} D^4 = \sum_{[i_1,i_2,i_3,i_4]} \frac{|[i_1,i_2,i_3,i_4]|}{2} [1 + \dagger] \mathcal{B}(i_1,i_2,i_3,i_4) \tag{15}$$

where $\dagger$ denotes Hermitian conjugation of everything that appears on the right, and the factor ${}^{|[i_1,i_2,i_3,i_4]|}/_2$ involving the cardinality of the class prevents from overcounting terms of the type $\mathcal{B}(i_1, i_2, i_2, i_1)$.
The truncated sum can be written explicitly in the following way:

$$\begin{aligned}
\frac{\partial}{\partial M_k} \operatorname{Tr} D^4 = & \\
& \sum_{\substack{i_4<i_1 \\ i_3<i_2}} [1+\dagger]\big(\mathcal{B}(i_1,i_2,i_3,i_4)+\mathcal{B}(i_1,i_3,i_2,i_4)\big)+ \\
& \sum_{\substack{i_4=i_1 \\ i_3<i_2}} [1+\dagger]\mathcal{B}(i_1,i_2,i_3,i_4) + \sum_{\substack{i_4<i_1 \\ i_3=i_2}} [1+\dagger]\mathcal{B}(i_1,i_2,i_3,i_4)+ \\
& \sum_{\substack{i_4=i_1 \\ i_3=i_2}} \mathcal{B}(i_1,i_2,i_3,i_4)
\end{aligned} \tag{16}$$

Moreover notice that the second line vanishes due to the properties of the ω matrices:

$$\operatorname{Tr}(\omega_{\sigma(i_1)}\omega_{\sigma(i_2)}\omega_{\sigma(j)}\omega_{\sigma(k)}) \sim \operatorname{Tr}(\omega_j\omega_k) = 0 \qquad \text{if} \;\; i_1 = i_2 \text{ and } j \neq k \tag{17}$$

for any permutation σ acting on $\{i_1, i_2, j, k\}$.
Therefore Eq.(16) simplifies to:

$$\begin{aligned}
\frac{\partial}{\partial M_k} \operatorname{Tr} D^4 = & \\
& \sum_{\substack{i_4<i_1 \\ i_3<i_2}} [1+\dagger]\big(\mathcal{B}(i_1,i_2,i_3,i_4)+\mathcal{B}(i_1,i_3,i_2,i_4)\big) + \sum_{i_1,i_2} \mathcal{B}(i_1,i_2,i_2,i_1)
\end{aligned} \tag{18}$$

which is a Hermitian matrix.

1.5 A general formula for every p

The first problem is to write $\operatorname{Tr} D^p$ in a useful form, along the lines of Eq.(10). $\operatorname{Tr} D^p$ expands to:

$$\begin{aligned}
\operatorname{Tr} D^p = \sum_{i_1 \dots i_p} \operatorname{Tr} \omega_{i_1} \dots \omega_{i_p} \cdot & \\
\operatorname{Tr} \big((M_{i_1} \otimes I + \epsilon_{i_1} I \otimes M_{i_1}^T) \dots (M_{i_p} \otimes I + \epsilon_{i_p} I \otimes M_{i_p}^T) \big) &
\end{aligned} \tag{19}$$

Ignoring (for now) the trace over the ω matrices, a typical term in the sum is:

$$\mathrm{Tr}\left(\epsilon_B A \otimes B^* + \epsilon_A B \otimes A^*\right) \tag{20}$$

where A and B are related to the product $M_{i_1} \dots M_{i_p}$ in the following way:

1. pick $r \geq 0$ numbers $k_1 < \dots < k_r$ from $\{1, \dots, p\}$ and call the remaining $p - r$ numbers $j_1 < \dots < j_{p-r}$;
2. define $A = M_{i_{k_1}} \dots M_{i_{k_r}}$ and $B = M_{i_{j_1}} \dots M_{i_{j_{p-r}}}$ (if $r = 0$, $A = I$);
3. define $\epsilon_A = \epsilon_{i_{k_1}} \dots \epsilon_{i_{k_r}}$ and $\epsilon_B = \epsilon_{i_{j_1}} \dots \epsilon_{i_{j_{p-r}}} = \epsilon_A \epsilon_{i_1} \dots \epsilon_{i_p}$.

In particular, a choice of A completely characterizes B.
By varying r from 0 to $\left[\frac{p}{2}\right]$ and summing over all possible choices of $k_1 \dots k_r$, every term in $\mathrm{Tr}\, D^p$ is generated.
One can verify that every term in Eq.(10) ($p = 4$) is of that type. For example:

$$\begin{aligned}
&\mathrm{Tr}\, M_{i_1}[\epsilon_{i_1} + \epsilon_{i_2}\epsilon_{i_3}\epsilon_{i_4} *]\, \mathrm{Tr}(M_{i_2} M_{i_3} M_{i_4}) = \\
&\qquad \epsilon_{i_2}\epsilon_{i_3}\epsilon_{i_4}\, \mathrm{Tr}\, M_{i_1}\, \mathrm{Tr}(M_{i_2} M_{i_3} M_{i_4})^* + \epsilon_{i_1}\, \mathrm{Tr}\, M_{i_1}\, \mathrm{Tr}(M_{i_2} M_{i_3} M_{i_4}) = \\
&\qquad \epsilon_{i_2}\epsilon_{i_3}\epsilon_{i_4}\, \mathrm{Tr}\, M_{i_1}\, \mathrm{Tr}(M_{i_2} M_{i_3} M_{i_4})^* + \epsilon_{i_1}\, \mathrm{Tr}(M_{i_1})^*\, \mathrm{Tr}(M_{i_2} M_{i_3} M_{i_4}) = \\
&\qquad \mathrm{Tr}\left(\epsilon_{i_2}\epsilon_{i_3}\epsilon_{i_4} M_{i_1} \otimes (M_{i_2} M_{i_3} M_{i_4})^* + \epsilon_{i_1} M_{i_2} M_{i_3} M_{i_4} \otimes M_{i_1}^*\right)
\end{aligned} \tag{21}$$

which is of the form of Eq.(20) upon identifying M_{i_1} with A and $M_{i_2} M_{i_3} M_{i_4}$ with B (in the second equality the reality of $\mathrm{Tr}\, M_{i_1}$ has been used).
A way of expressing $\mathrm{Tr}\, B$ given A is using a modified derivative operator D_i defined as:

$$\mathrm{D}_i \equiv \mathrm{Tr}\ \circ \frac{\partial}{\partial M_i} \tag{22}$$

which allows to write:

$$A = M_{i_{k_1}} \dots M_{i_{k_r}} \implies \mathrm{Tr}\, B = \mathrm{D}_{i_{k_r}} \dots \mathrm{D}_{i_{k_1}}\, \mathrm{Tr}(M_{i_1} \dots M_{i_p}). \tag{23}$$

Therefore Eq.(20) becomes:

$$\begin{aligned}
&\epsilon_A [1 + \epsilon_{i_1} \dots \epsilon_{i_p} *](\mathrm{Tr}\, A)^*\, \mathrm{Tr}\, B = \\
&\quad \epsilon_{i_{k_1}} \dots \epsilon_{i_{k_r}} [1 + \epsilon_{i_1} \dots \epsilon_{i_p} *](\mathrm{Tr}\, M_{i_{k_1}} \dots M_{i_{k_r}})^* \left(\mathrm{D}_{i_{k_r}} \dots \mathrm{D}_{i_{k_1}}\, \mathrm{Tr}(M_{i_1} \dots M_{i_p})\right).
\end{aligned} \tag{24}$$

There are some special cases that make the expression simpler, namely:

1. $r = 0$ gives a factor $\mathrm{Tr}\, I = n$;
2. $r = 1, 2$ make $\mathrm{Tr}\, A$ real;
3. $p - r = 1, 2$ (which can only occur for $p = 2, 4$) make $\mathrm{Tr}\, B$ real.

Putting everything together, $\mathrm{Tr}\, D^p$ can be written as:

$$\mathrm{Tr}\, D^p = \sum_{i_1 \dots i_p} \mathrm{Tr}\ \omega_{i_1} \dots \omega_{i_p} \left[\sum_{r=0}^{[\frac{p}{2}]} \sum_{k_1 < \dots < k_r = 1}^{p} \epsilon_{i_{k_1}} \dots \epsilon_{i_{k_r}} [1 + \epsilon_{i_1} \dots \epsilon_{i_p} *] \right.$$
$$\left. (\mathrm{Tr}\, M_{i_{k_1}} \dots M_{i_{k_r}})^* \big(\mathrm{D}_{i_{k_r}} \dots \mathrm{D}_{i_{k_1}} \mathrm{Tr}(M_{i_1} \dots M_{i_p}) \big) \right]. \tag{25}$$

where:

$$r = 0 \quad \longrightarrow \quad n[1 + \epsilon_{i_1} \dots \epsilon_{i_p} *]\, \mathrm{Tr}(M_{i_1} \dots M_{i_p}) \tag{26}$$

$$r = 1 \quad \longrightarrow \quad \sum_{k_1=0}^{p} \epsilon_{i_{k_1}} \mathrm{Tr}(M_{i_{k_1}})[1 + \epsilon_{i_1} \dots \epsilon_{i_p} *]\, \mathrm{D}_{i_{k_1}} \mathrm{Tr}(M_{i_1} \dots M_{i_p}) \tag{27}$$

$$r = 2 \quad \longrightarrow \quad \sum_{k_1 < k_2 = 0}^{p} \epsilon_{i_{k_1}} \epsilon_{i_{k_2}} \mathrm{Tr}(M_{i_{k_1}} M_{i_{k_2}})[1 + \epsilon_{i_1} \dots \epsilon_{i_p} *]\, \mathrm{D}_{i_{k_2}} \mathrm{D}_{i_{k_1}} \mathrm{Tr}(M_{i_1} \dots M_{i_p}). \tag{28}$$