XY CHAIN COMPUTATION

1. Background

Given a Hamiltonian $\mathcal{H}$ We wish to construct a factorisation

$$\mathcal{H} = KhK^\dagger \tag{1}$$

where h is a sum of commutative Pauli strings.
This lends itself to efficient Hamiltonian simulation via

$$e^{-i\mathcal{H}t} = Ke^{-iht}K^\dagger \tag{2}$$

By the work of Earp and Pachos which extended on from Khaneja and Glaser, we achieve the following:
For Cartan decomposition $\mathfrak{g} = \mathfrak{k} \bigoplus \mathfrak{p}$, and Cartan subalgebra $\mathfrak{h}$, with corresponding Lie groups **G,K,M,H**

$$\mathfrak{p} = \bigcup_{K \in \mathbf{K}} \mathrm{Ad}_K(\mathfrak{h}) \tag{3}$$

That is, for $p \in \mathfrak{p}$, $\exists K_1^\dagger \in \mathbf{K}$ whose action rotates p onto an element h of the Cartan subalgebra $\mathfrak{h}$.
In order to prove this, they take an arbitrary $v \in$
fh which generates a dense subgroup $\exp(tv) \subseteq \mathbf{H}$ and define the function

$$\begin{aligned} f_{v,p} &= f : \mathbf{K} \to \mathbb{R} \\ K &\to f(K) = \langle v, \mathrm{Ad}_K(p) \rangle \end{aligned} \tag{4}$$

where $\langle a, b \rangle = \mathrm{tr}(ad_a ad_b)$ is the Killing form on $\mathfrak{g}$.
Then for some locally extremising K_1, we have that

$$0 = \left.\frac{d}{dt}\right|_{t=0} f(e^{tk}K_1) = \cdots = \mathrm{tr}(\mathrm{ad}_{[h,v]}\mathrm{ad}_k) \iff \langle [h,v], k \rangle = 0 \quad \forall k \in \mathfrak{k} \tag{5}$$

where $h = \mathrm{Ad}_{K_1}(p)$.
Since the Killing form is non-degenerate on $\mathfrak{k}$, we must have that $[h, v] = 0$.
The paper then states that this implies $h \in \mathfrak{h}$ because v is centralised by $\mathfrak{h}$. Is it true that the only elements which centralise a given $v \in \mathfrak{h}$ are other elements of $\mathfrak{h}$? This doesn't seem right... Perhaps you can advise
Given this holds, we have shown that

$$p = \mathrm{Ad}_{K_1^\dagger}(h) \tag{6}$$

So the idea for our Hamiltonian simulation is to choose $p = \mathcal{H} \in \mathfrak{p}$ and compute such a factorisation.

2. Implementation

The first challenge is to construct a suitable Cartan decomposition such that $\mathcal{H} \in \mathfrak{p}$.
Cartan decompositions of a real semisimple Lie algebra are in bijection with Cartan involutions [Anthony W. Knapp, Lie groups beyond an introduction, page 360], where we set the +1 eigenspace to be $\mathfrak{k}$ and the -1 eigenspace to be $\mathfrak{p}$.
So it suffices to choose an involution ϕ such that the components of $\mathcal{H}$ are in the -1 eigenspace.
From this we then identify a Cartan subalgebra $\mathfrak{h}$.

Kokcu et al's approach is to then choose an arbitrary $v \in \mathfrak{h}$ whose exponential map is dense in $\mathbf{H}$, that is $v = \sum_j \alpha_j h_j$ with α_j mutually irrational, and then define the function

$$f(\theta) = \langle K(\theta) v K^\dagger(\theta), \mathcal{H} \rangle \tag{7}$$

where

$$K(\theta) = \prod_j e^{i\theta_j k_j} \tag{8}$$

The key result of the paper is that for any θ_C that locally extremises $f(\theta)$, we have that

$$K^\dagger(\theta_C) \mathcal{H} K(\theta_C) = h \in \mathfrak{h} \tag{9}$$

The novel insight is that the form of K in (8) is sufficient, despite not necessarily spanning $\mathbf{K}$.
In their proof, the constraints on the of inner product is that it must be a non-degenerate invariant bilinear form, so a scalar multiple of the Killing form is sufficient.

$$\langle A, B \rangle = \frac{1}{2^n} \operatorname{Trace}(AB) \tag{10}$$

They then implement a BFGS optimisation routine to find θ_C and finally compute $h = K_C^\dagger \mathcal{H} K_C$ to obtain the parameters for the decomposition (1).

3. Our Hamiltonian

We shall focus our attention to the Kitaev chain for n even

$$\mathcal{H}(a) = \sum_{j=1}^{n-1} a_j X_j Y_{j+1} \tag{11}$$

For $a < b$, let us denote the element $X_a Z^{\otimes b-a-1} Y_b$ as $\gamma_{a,b}$, and for ease of notation identify $\gamma_{a,b} = \gamma_{b,a}$ It is useful to establish the commutation relations that for $a < b < c$

$$\left[\frac{i}{2}\gamma_{a,b}, \frac{i}{2}\gamma_{b,c}\right] = \frac{i}{2}\gamma_{a,c}, \qquad \left[\frac{i}{2}\gamma_{a,c}, \frac{i}{2}\gamma_{a,b}\right] = \frac{i}{2}\gamma_{b,c}, \qquad \left[\frac{i}{2}\gamma_{b,c}, \frac{i}{2}\gamma_{a,c}\right] = \frac{i}{2}\gamma_{a,b}. \tag{12}$$

Then the Lie algebra generated by $\{\gamma_{j,j+1} \mid j \in 1, ..., n-1\}$ is

$$\mathfrak{g}(i\mathcal{H}) = \mathrm{span}_{\mathbb{R}}\{i\gamma_{a,b} \mid 1 \leq a < b \leq n\} \tag{13}$$

Using the Cartan involution

$$\phi(A) = X^{\otimes n} A X^{\otimes n} \tag{14}$$

We obtain a Cartan decomposition $\mathfrak{g} = \mathfrak{k} \oplus \mathfrak{p}$ where

$$\mathfrak{k} = \mathrm{span}_{\mathbb{R}}\{i\gamma_{a,b} \mid a \equiv b \pmod 2, \quad 1 \leq a < b \leq n\} \tag{15}$$

$$\mathfrak{p} = \mathrm{span}_{\mathbb{R}}\{i\gamma_{a,b} \mid a \equiv b+1 \pmod 2, \quad 1 \leq a < b \leq n\} \tag{16}$$

And choose the Cartan subalgebra

$$\mathfrak{h} = \mathrm{span}_{\mathbb{R}}\{i\gamma_{j,j+1} \mid j \equiv 1 \pmod 2, \quad 1 \leq j \leq n-1\} \tag{17}$$

A natural splitting arises $\mathfrak{k} = \mathfrak{k}_{even} \oplus \mathfrak{k}_{odd}$

$$\mathfrak{k}_{even} = \mathrm{span}_{\mathbb{R}}\{i\gamma_{ab} \mid a \equiv b \equiv 0 \pmod 2\}, \qquad \mathfrak{k}_{odd} = \mathrm{span}_{\mathbb{R}}\{i\gamma_{ab} \mid a \equiv b \equiv 1 \pmod 2\} \tag{18}$$

Such that $[\mathfrak{k}_{even}, \mathfrak{k}_{odd}] = 0$.

$$\mathfrak{g} \cong \mathfrak{so}(n) \qquad \mathfrak{k} = \mathfrak{k}_{even} \oplus \mathfrak{k}_{odd} \cong \mathfrak{so}(n/2) \oplus \mathfrak{so}(n/2) \tag{19}$$

$$|\mathfrak{g}| = \binom{n}{2} \qquad |\mathfrak{k}| = 2\binom{n/2}{2} \qquad |\mathfrak{p}| = \frac{n^2}{4} \tag{20}$$

4. The action of K

Define the action of $\mathfrak{k}$ on $\mathfrak{p}$ by

$$\begin{aligned} &A(\theta) : \mathfrak{k} \to GL(\mathfrak{p}) \\ &A_{c,d}(\theta) : \gamma_{a,b} \mapsto e^{i\theta\gamma_{c,d}}\gamma_{a,b}e^{-i\theta\gamma_{c,d}} \end{aligned} \tag{21}$$

To show this is in fact a linear map, the conjugation can be computed to be

$$A_{c,d}(\theta)(\gamma_{a,b}) = \begin{cases} \gamma_{a,b} & [\gamma_{c,d}, \gamma_{a,b}] = 0 \\ \cos(2\theta)\gamma_{a,b} - \frac{1}{2i}\sin(2\theta)[\gamma_{c,d}, \gamma_{a,b}] & \{\gamma_{c,d}, \gamma_{a,b}\} = 0 \end{cases} \tag{22}$$

By the commutation relations (17), $[\gamma_{c,d}, \gamma_{a,b}] \neq 0$ if and only if $|\{a, b, c, d\}| = 3$ and further

$$[i\gamma_{c,d}, i\gamma_{b,c}] = (-1)^{1+\mathbb{1}(c<b<d)} 2i\gamma_{b,d} \tag{23}$$

$$[i\gamma_{c,d}, i\gamma_{b,d}] = (-1)^{\mathbb{1}(c<b<d)} 2i\gamma_{b,c} \tag{24}$$

By vectorising $\mathfrak{p}$ as

$$p = \sum_{\gamma_{a,b} \in \mathfrak{p}} \alpha_{a,b}\gamma_{a,b} \mapsto M_p = \begin{bmatrix} \alpha_{1,2} & \alpha_{3,2} & \dots & \alpha_{n-1,2} \\ \alpha_{1,4} & \alpha_{3,4} & \dots & \alpha_{n-1,4} \\ \vdots & & & \vdots \\ \alpha_{1,n} & \alpha_{3,n} & \dots & \alpha_{n-1,n} \end{bmatrix} \tag{25}$$

We identify that $M_{\mathfrak{h}}$ is the set of diagonal matrices.

For $\gamma_{a,b} \in \mathfrak{k}_{odd}$ and $\gamma_{c,d} \in \mathfrak{k}_{even}$ and where $c = \cos(2\theta)$ and $s = \sin(2\theta)$

(26)

$$A_{a,b}(\theta)p \mapsto \begin{bmatrix} \alpha_{1,2} & \dots & c\alpha_{a,2} + s\alpha_{b,2} & \dots & c\alpha_{b,2} - s\alpha_{a,2} & \dots & \alpha_{n-1,2} \\ \vdots & & \vdots & & \vdots & & \vdots \\ \alpha_{1,a-1} & \dots & c\alpha_{a,a-1} + s\alpha_{b,a-1} & \dots & c\alpha_{b,a-1} - s\alpha_{a,a-1} & \dots & \alpha_{n-1,a-1} \\ \alpha_{1,a+1} & \dots & c\alpha_{a,a+1} - s\alpha_{b,a+1} & \dots & c\alpha_{b,a+1} + s\alpha_{a,a+1} & \dots & \alpha_{n-1,a+1} \\ \vdots & & \vdots & & \vdots & & \vdots \\ \alpha_{1,b-1} & \dots & c\alpha_{a,b-1} - s\alpha_{b,b-1} & \dots & c\alpha_{b,b-1} + s\alpha_{a,b-1} & \dots & \alpha_{n-1,b-1} \\ \alpha_{1,b+1} & \dots & c\alpha_{a,b+1} + s\alpha_{b,b+1} & \dots & c\alpha_{b,b+1} - s\alpha_{a,b+1} & \dots & \alpha_{n-1,b+1} \\ \vdots & & \vdots & & \vdots & & \vdots \\ \alpha_{1,n} & \dots & c\alpha_{a,n} + s\alpha_{b,n} & \dots & c\alpha_{b,n} - s\alpha_{a,n} & \dots & \alpha_{n-1,n} \end{bmatrix}$$

$$A_{c,d}(\theta)p \mapsto \begin{bmatrix} \alpha_{1,2} & \dots & \alpha_{c-1,2} & \alpha_{c+1,2} & \dots & \alpha_{d-1,2} & \alpha_{d+1,2} & \dots & \alpha_{n-1,2} \\ \vdots & \vdots & & \vdots & & & & & \\ c\alpha_{1,c} + s\alpha_{1,d} & \dots & c\alpha_{c-1,c} + s\alpha_{c-1,d} & c\alpha_{c+1,c} - s\alpha_{c+1,d} & \dots & c\alpha_{d-1,c} - s\alpha_{d-1,d} & c\alpha_{d+1,c} + s\alpha_{d+1,d} & \dots & c\alpha_{n-1,c} + s\alpha_{n-1,d} \\ \vdots & \vdots & & \vdots & & & & & \\ c\alpha_{1,d} - s\alpha_{1,c} & \dots & c\alpha_{c-1,d} - s\alpha_{c-1,c} & c\alpha_{c+1,d} + s\alpha_{c+1,c} & \dots & c\alpha_{d-1,d} + s\alpha_{d-1,c} & c\alpha_{d+1,d} - s\alpha_{d+1,c} & \dots & c\alpha_{n-1,2} - s\alpha_{n-1,c} \\ \vdots & \vdots & & \vdots & & & & & \\ \alpha_{1,n} & \dots & \alpha_{c-1,n} & \alpha_{c+1,n} & \dots & \alpha_{d-1,2} & \alpha_{d+1,n} & \dots & \alpha_{n-1,n} \end{bmatrix}$$

Note that these can be computed in $O(n)$ operations and there are $O(n^2)$ such matrices.

5. Finding θ_C

- $\frac{\partial f}{\partial \theta} = 0$ - I elaborate in section 8 why I don't think this will prove to be a good approach
- Riemannian gradient flow
- BFGS
- v as a weighted trace, the proof requires the weightings to be mutually irrational in general, is this true for our case? Or could the unweighted trace suffice?
- The action of $A_{cd}(\theta)$ preserves the L2 norm of M_p, so $\sum_{j=1}^{n-1} a_i^2 = \sum_{j=1}^{n/2} \beta_j^2$ where $h = \sum_{j=1}^{n/2} \beta_j \gamma_{2j-1,2j}$
- Could we write an algorithm to manually apply conjugations until we diagonalise this matrix? This may involve additional gates but also solve the problem analytically.

6. Finding h

Upon obtaining θ_C such that $A(-\theta_C)\mathcal{H} = K_C^\dagger \mathcal{H} K_C \in \mathfrak{h}$, we can compute $M_{A(-\theta_C)\mathcal{H}} = M_h \in GL(\mathfrak{p})$ in $O(n^3)$ steps.
It is then easy to verify that this is diagonal and read off the diagonal entries.

7. Questions

(1) 2x2 Jordan Block?
(2) Prove $\mathfrak{g} \equiv \mathfrak{so}(n)$
(3) Is there a better method than BFGS?
(4) A lot of recent papers discuss Barren Plateaus where local to the extremum f becomes exponentially flat with n.
Might we encounter this? Larocca and Ragone
(5) There's some related literature on Riemannian gradient flow - worth looking into? Wiersema and Killoran
(6) Do we need v? It seems slightly 'clunky'
$M_{\mathcal{H}}$ is an upper bidiagonal matrix and M_h is diagonal. Our actions are row and element operations, but not quite the type which preserve the determinant - is there a volume form which is conserved?

8. Likely failed ideas

8.1. $\frac{\partial f}{\partial \theta}$. Using the identity

$$\frac{d}{d\lambda}\left(e^{\lambda S} T e^{-\lambda S}\right) = e^{\lambda S}[S,T]e^{-\lambda S} \tag{27}$$

We could consider pursuing an exact formula for $\frac{\partial f}{\partial \theta_j}$.
Write $K(\theta) = K_1 e^{i\theta_j k_j} K_2$.
Then

$$\frac{\partial f}{\partial \theta_j} = \langle i K_1 e^{i\theta_j k_j}[k_j, K_2 v K_2^\dagger] e^{-i\theta_j k_j} K_1^\dagger, \mathcal{H}\rangle \tag{28}$$

A useful result may be that for Pauli strings

$$[A,\, e^{i\theta B} C e^{-i\theta B}] \;=\; \begin{cases} e^{i\theta B}\,[A,C]\,e^{-i\theta B}, & [A,B]=0, \\ e^{i\theta B}\big(\cos(2\theta)\,[A,C] + i\sin(2\theta)\,[AB,C]\big)e^{-i\theta B}, & \{A,B\}=0 \end{cases} \tag{29}$$

However this would suggest that computing the derivative is of the same order of complexity as computing f, so I do not see that this will lead to an improvement.