XY-4-Chain

Basics

Hamiltonian	$\mathcal{H}(a) = a_1X_1Y_2 + a_2X_2Y_3 + a_3X_3Y_4 = \sum_{j=1}^{3} a_jX_jY_{j+1}$	(1)
Lie Algebra	$\mathfrak{g}(\mathcal{H}) = \text{span}\{X_1Y_2, X_2Y_3, X_3Y_4, X_1Z_2Y_3, X_2Z_3Y_4, X_1Z_2Z_3Y_4\}$	(2)
Involution	$\phi(A) = X^{\otimes 4}AX^{\otimes 4}$	(3)
Cartan Decomposition	$\mathfrak{k} = \text{span}\{X_1Z_2Y_3, X_2Z_3Y_4\}$	(4)
	$\mathfrak{m} = \text{span}\{X_1Y_2, X_2Y_3, X_3Y_4, X_1Z_2Z_3Y_4\}$	(5)
Cartan Subalgebras	$\mathfrak{h}_1 = \text{span}\{X_1Y_2, X_3Y_4\}$	(6)
	$\mathfrak{h}_2 = \text{span}\{X_2Y_3, X_1Z_2Z_3Y_4\}$	(7)
Parametrisations	$K(\theta) = e^{i\theta_1X_1Z_2Y_3}e^{i\theta_2X_2Z_3Y_4}$	(8)
	$v_1(\alpha_1, \alpha_2) = \alpha_1X_1Y_2 + \alpha_2X_3Y_4$	(9)
	$v_2(\alpha_1, \alpha_2) = \alpha_1X_2Y_3 + \alpha_2X_1Z_2Z_3Y_4$	(10)
	$h_1(\beta_1, \beta_2) = \beta_1X_1Y_2 + \beta_2X_3Y_4$	(11)
	$h_2(\beta_1, \beta_2) = \beta_1X_2Y_3 + \beta_2X_1Z_2Z_3Y_4$	(12)
Cost function (Killing form)	$f_j(\theta) = \langle K(\theta)v_j(\alpha_1, \alpha_2)K(\theta)^\dagger, \mathcal{H}\rangle = \frac{1}{2^n}\text{Tr}(Kv_jK^\dagger\mathcal{H})$	(13)
Hamiltonian Decomposition	$\mathcal{H} = KhK^\dagger$	(14)

Note that our involution ϕ is such that $\mathfrak{m}$ is the span of elements $X_aZ_{a+1}...Z_{b-1}Y_b$ such that $b-a$ is odd
Further, our inner product is scaled such that the Pauli strings form an orthonormal set

Our decomposition relies on two key theorems

Theorem 1 *$\mathcal{H} = Kh_jK^\dagger$ for some $K \in e^{i\mathfrak{k}}$ and $h_j \in \mathfrak{h}_j$*

Theorem 2 *If e^{itv_j} is dense in $e^{i\mathfrak{h}_j}$, then local extremum θ_C of $f_j(\theta)$ satisfies $K_C^\dagger\mathcal{H}K_C \in \mathfrak{h}_j$*

The Hamiltonian

For our 4-qubit system, it is possible to directly compute the eigenvalues
We see that they are

$$\pm\sqrt{a_2^2 + (a_1 - a_3)^2}, \qquad \pm\sqrt{a_2^2 + (a_1 + a_3)^2} \tag{15}$$

each with multiplicity 4
We will see that this informs the form of h_j

Commutation Relations

Let us relabel

$$A_\pm = \frac{1}{2}(X_1Z_2Y_3 \pm X_2Z_3Y_4) \qquad B_\pm = \frac{1}{2}(X_1Y_2 \pm X_3Y_4) \qquad C_\pm = \frac{1}{2}(X_2Y_3 \pm X_1Z_2Z_3Y_4) \tag{16}$$

and compute the commutation relations

$[A,B]$	B_+	B_-
A_+	0	$-2iC_-$
A_-	$-2iC_+$	0

$[A,C]$	C_+	C_-
A_+	0	$2iB_-$
A_-	$2iB_+$	0

So using the identity

$$\frac{d}{d\lambda}\left(e^{\lambda S}Te^{-\lambda S}\right) = e^{\lambda S}[S,T]e^{-\lambda S} \tag{17}$$

And by considering the non-degenerate transformations

$$(\theta_1,\theta_2) \to \left(\frac{\theta_1+\theta_2}{2}, \frac{\theta_1-\theta_2}{2}\right) \qquad (\alpha_1,\alpha_2) = \frac{\alpha_1+\alpha_2}{2}(1,1) + \frac{\alpha_1-\alpha_2}{2}(1,-1) \tag{18}$$

We can rewrite our optimality condition

$$\begin{aligned} \frac{i}{2}\frac{\partial f_1(1,-1)}{\partial(\theta_1+\theta_2)/2} &= f_2(1,-1) = 0 \\ \frac{i}{2}\frac{\partial f_1(1,1)}{\partial(\theta_1-\theta_2)/2} &= f_2(1,1) = 0 \end{aligned} \tag{19}$$

That is

$$\langle X_2Y_3 \pm X_1Z_2Z_3Y_4, K(\theta)^\dagger \mathcal{H} K(\theta)\rangle = 0 \tag{20}$$

And for such a θ, we have that h_1 is given by

$$\begin{aligned} \beta_1 &= \langle X_1Y_2, K(\theta)^\dagger \mathcal{H} K(\theta)\rangle = f_1(1,0) \\ \beta_2 &= \langle X_3Y_4, K(\theta)^\dagger \mathcal{H} K(\theta)\rangle = f_1(0,1) \end{aligned} \tag{21}$$

A couple of things to note:

1. A symmetric argument holds for h_2
2. Our commutation relations also give us that

$$\frac{\partial^2 f_j}{\partial \theta_k^2} = 4f_j \qquad \forall j,k \tag{22}$$

   and so, unless $f_j(\theta) = 0$, we can be sure that this is a local extremum
3. The form $\langle X_2Y_3 \pm X_1Z_2Z_3Y_4, K(\theta)^\dagger \mathcal{H} K(\theta)\rangle = 0$ is nice

Symbolic Computation

We can symbolically compute $\langle X_1 Y_2 \pm X_3 Y_4, K^\dagger \mathcal{H} K \rangle$ and $\langle X_2 Y_3 \pm X_1 Z_2 Z_3 Y_4, K^\dagger \mathcal{H} K \rangle$

$$f_1(1,1) = a_2 \sin(2\theta_1 - 2\theta_2) + (a_1 + a_3)\cos(2\theta_1 - 2\theta_2) \tag{23}$$
$$f_1(1,-1) = a_2 \sin(2\theta_1 + 2\theta_2) + (a_1 - a_3)\cos(2\theta_1 + 2\theta_2) \tag{24}$$
$$f_2(1,1) = a_2 \cos(2\theta_1 - 2\theta_2) - (a_1 + a_3)\sin(2\theta_1 - 2\theta_2) \tag{25}$$
$$f_2(1,-1) = a_2 \cos(2\theta_1 + 2\theta_2) - (a_1 - a_3)\sin(2\theta_1 + 2\theta_2) \tag{26}$$

So we can factorise $\mathcal{H}$ into $\mathfrak{h}_1$ via

$$\theta_1 + \theta_2 = \frac{1}{2}\arctan\left(\frac{a_2}{a_1 - a_3}\right) + \frac{\pi}{2}\mathbb{1}[a_1 - a_3 < 0] \tag{27}$$
$$\theta_1 - \theta_2 = \frac{1}{2}\arctan\left(\frac{a_2}{a_1 + a_3}\right) + \frac{\pi}{2}\mathbb{1}[a_1 + a_3 < 0] \tag{28}$$
$$\beta_1 + \beta_2 = \sqrt{a_2^2 + (a_1 + a_3)^2} \tag{29}$$
$$\beta_1 - \beta_2 = \sqrt{a_2^2 + (a_1 - a_3)^2} \tag{30}$$

Or instead into $\mathfrak{h}_2$ via

$$\theta_1 + \theta_2 = -\frac{1}{2}\arctan\left(\frac{a_1 - a_3}{a_2}\right) + \frac{\pi}{2}\mathbb{1}[a_2 < 0] \tag{31}$$
$$\theta_1 - \theta_2 = -\frac{1}{2}\arctan\left(\frac{a_1 + a_3}{a_2}\right) + \frac{\pi}{2}\mathbb{1}[a_2 < 0] \tag{32}$$
$$\beta_1 + \beta_2 = \sqrt{a_2^2 + (a_1 + a_3)^2} \tag{33}$$
$$\beta_1 - \beta_2 = \sqrt{a_2^2 + (a_1 - a_3)^2} \tag{34}$$

XY-6-Chain

Basics

$$\mathcal{H}(\vec{a}) = a_1X_1Y_2 + a_2X_2Y_3 + a_3X_3Y_4 + a_4X_4Y_5 + a_5X_5Y_6 = \sum_{j=1}^{5} a_jX_jY_{j+1} \tag{35}$$

$$\begin{aligned}\mathfrak{g}(\mathcal{H}) = \mathrm{span}\{&X_1Y_2, X_2Y_3, X_3Y_4, X_4Y_5, X_5Y_6,\\ &X_1Z_2Y_3, X_2Z_3Y_4, X_3Z_4Y_5, X_4Z_5Y_6, X_1Z_2Z_3Y_4, X_2Z_3Z_4Y_5, X_3Z_4Z_5Y_6,\\ &X_1Z_2Z_3Z_4Y_5, X_2Z_3Z_4Z_5Y_6, X_1Z_2Z_3Z_4Z_5Y_6\}\end{aligned} \tag{36}$$

$$\phi(A) = X^{\otimes 6}AX^{\otimes 6} \tag{37}$$

$$\mathfrak{k} = \mathrm{span}\{X_1Z_2Y_3, X_2Z_3Y_4, X_3Z_4Y_5, X_4Z_5Y_6, X_1Z_2Z_3Z_4Y_5, X_2Z_3Z_4Z_5Y_6\} \tag{38}$$

$$\mathfrak{m} = \mathrm{span}\{X_1Y_2, X_2Y_3, X_3Y_4, X_4Y_5, X_5Y_6, X_1Z_2Z_3Y_4, X_2Z_3Z_4Y_5, X_3Z_4Z_5Y_6, X_1Z_2Z_3Z_4Z_5Y_6\} \tag{39}$$

$$\mathfrak{h}_1 = \mathrm{span}\{X_1Y_2, X_3Y_4, X_5Y_6\} \tag{40}$$

$$\mathfrak{h}_2 = \mathrm{span}\{X_3Y_4, X_2Z_3Z_4Y_5, X_1Z_2Z_3Z_4Z_5Y_6\} \tag{41}$$

$$K(\vec{\theta}) = e^{i\theta_1X_1Z_2Y_3}e^{i\theta_2X_2Z_3Y_4}e^{i\theta_3X_3Z_4Y_5}e^{i\theta_4X_4Z_5Y_6}e^{i\theta_5X_1Z_2Z_3Z_4Y_5}e^{i\theta_6X_2Z_3Z_4Z_5Y_6} \tag{42}$$

$$h_1 = \beta_1X_1Y_2 + \beta_2X_3Y_4 + \beta_3X_5Y_6 \tag{43}$$

$$h_2 = \beta_1X_1Z_2Z_3Z_4Z_5Y_6 + \beta_2X_2Z_3Z_4Y_5 + \beta_3X_3Y_4 \tag{44}$$

$$h_3 = \beta_1X_2Y_3 + \beta_2X_1Z_2Z_3Y_4 + \beta_3X_5Y_6 \tag{45}$$

$$h_4 = \beta_1X_1Y_2 + \beta_2X_3Z_4Z_5Y_6 + \beta_3X_4Y_5 \tag{46}$$

Basics ver 2

For ease, let us denote $X_a Z_{a+1} ... Z_{b-1} Y_b$ as (ab)

$$\mathcal{H}(\vec{a}) = a_1(12) + a_2(23) + a_3(34) + a_4(45) + a_5(56) = \sum_{j=1}^{5} a_j(j \quad j+1) \tag{47}$$

$$\begin{aligned} \mathfrak{g}(\mathcal{H}) &= \text{span}\{(12),(23),(34),(45),(56),(13),(24),(35),(46),(14),(25),(36),(15),(26),(16)\} \\ &= \{(ab) \mid 1 \leq a < b \leq 6\} \end{aligned} \tag{48}$$

$$\phi(A) = X^{\otimes 6} A X^{\otimes 6} \tag{49}$$

$$\mathfrak{k} = \text{span}\{(13),(24),(35),(46),(15),(26)\} = \{(ab) \in \mathfrak{g} \mid b-a \text{ even}\} \tag{50}$$

$$\mathfrak{m} = \text{span}\{(12),(23),(34),(45),(56),(14),(25),(36),(16)\} = \{(ab) \in \mathfrak{g} \mid b-a \text{ odd}\} \tag{51}$$

$$K(\vec{\theta}) = e^{i\theta_1(13)} e^{i\theta_2(24)} e^{i\theta_3(35)} e^{i\theta_4(46)} e^{i\theta_5(15)} e^{i\theta_6(26)} \tag{52}$$

$$ \tag{53}$$

$$\mathfrak{h}_1 = \text{span}\{(12),(34),(56)\} \tag{54}$$

$$\mathfrak{h}_2 = \text{span}\{(34),(25),(16)\} \tag{55}$$

$$\mathfrak{h}_3 = \text{span}\{(12),(36),(45)\} \tag{56}$$

$$\mathfrak{h}_4 = \text{span}\{(23),(14),(56)\} \tag{57}$$

$$\mathfrak{h}_5 = \text{span}\{(14),(25),(36)\} \tag{58}$$

$$\mathfrak{h}_6 = \text{span}\{(16),(23),(45)\} \tag{59}$$

$$ \tag{60}$$

$$h_1 = \beta_1(12) + \beta_2(34) + \beta_3(56) \tag{61}$$

$$h_2 = \beta_1(16) + \beta_2(25) + \beta_3(34) \tag{62}$$

$$h_3 = \beta_1(12) + \beta_2(36) + \beta_3(45) \tag{63}$$

$$h_4 = \beta_1(23) + \beta_2(14) + \beta_3(56) \tag{64}$$

$$h_5 = \beta_1(14) + \beta_2(25) + \beta_3(36) \tag{65}$$

The Hamiltonian

Matlab timed out trying to compute the eigenvalues

Commutation Relations

Note that the actions of $\mathfrak{k}$ on $\mathfrak{h}_1$ act as involutions (up to scalar)
So once again we have $\frac{\partial^2 f}{\partial \theta_j^2} = 4f$ for all j
Which would suggest we are still working with cos and sin of 2(+- comb of thetas)
Is there some sort of inner product we can apply where each of these terms would be orthogonal?

First, it's a good idea to generalise the commutations, for $a < b < c < d$

$$[ab, cd] = 0 \tag{66}$$
$$[ac, bd] = 0 \tag{67}$$
$$[ad, bc] = 0 \tag{68}$$
$$[ab, ac] = 2i(bc) \tag{69}$$
$$[ac, bc] = 2i(ab) \tag{70}$$
$$[ab, bc] = -2i(ac) \tag{71}$$

I'll have a look at eigen-esque things, my inital idea is

- $(13) \pm (24)$ etc
- Then $\frac{\partial}{\partial(\theta_1+\theta_2)} \langle \gamma_1(12+34-56)+\gamma_2(-12+34+56)+\gamma_3(12-34+56), K^\dagger \mathcal{H} K\rangle = 4i(\gamma_2-\gamma_3)\langle (14-23), K^\dagger \mathcal{H} K\rangle$ etc
- So to find our θ_C, it suffices to find $\langle \_\_\_, K^\dagger \mathcal{H} K\rangle = 0$ for $(14 \pm 23), (36 \pm 45), (25 \pm 16)$

$\mathfrak{k}$	13	24	35	46	15	26
13	0	0	-2i(15)	0	2i(35)	0
24	0	0	0	-2i(26)	0	2i(46)
35	2i(15)	0	0	0	-2i(13)	0
46	0	2i(26)	0	0	0	-2i(24)
15	-2i(35)	0	2i(13)	0	0	0
26	0	-2i(46)	0	2i(24)	0	0

$\mathfrak{h}_1$	12+34-56	-12+34+56	12-34+56	Cartan
13+24	0	4i(14-23)	-4i(14-23)	4
13-24	-4i(14+23)	0	0	4
35+46	-4i(36-45)	0	4i(36-45)	3
35-46	0	-4i(36+45)	0	3
15+26	4i(25-16)	-4i(25-16)	0	2
15-26	0	0	-4i(25+16)	2

$\mathfrak{h}_1$	12	34	56	coeff	Cartan
13	23	14	0	-2i	4
24	14	23	0	2i	4
35	0	45	36	-2i	3
46	0	36	45	2i	3
15	25	0	16	-2i	2
26	16	0	25	2i	2

$\mathfrak{h}_2$	16	25	34	coeff	Cartan
13	36	0	14		5
24	0	45	23		6
35	0	23	45		6
46	14	0	36		5
15	56	12	0	2i	1
26	12	56	0	-2i	1

$\mathfrak{h}_3$	12	36	45	coeff	Cartan
13	23	16	0		6
24	14	0	25		5
35	0	56	34	2i	1
46	0	34	56	-2i	1
15	25	0	14		5
26	16	23	0		6

$\mathfrak{h}_4$	23	14	56	coeff	Cartan
13	12	34	0	2i	1
24	34	12	0	-2i	1
35	25	0	36		5
46	0	16	45		6
15	0	45	16		6
26	36	0	25		5

$\mathfrak{h}_5$	14	25	36	coeff	Cartan
13	34	0	16		2
24	12	45	0		3
35	0	23	56		4
46	16	0	34		2
15	45	12	0		3
26	0	56	23		4

$\mathfrak{h}_6$	16	23	45	coeff	Cartan
13	36	12	0		3
24	0	34	25		2
35	0	25	34		2
46	14	0	56		4
15	56	0	14		4
26	12	36	0		3