Perturbation Theory

So far, we have developed a very general theory of what constitutes analogue Hamiltonian simulation. But these general characterisation theorems do not tell us how to construct new simulations, only what mathematical form they must take and what properties they will have if we do construct one.

One important way (not the only one – see Tamara's lectures) to construct interesting simulations is via (rigorous) perturbation theory.

In perturbation theory, generally we have a strong and a weak term in a Hamiltonian, and we want to derive an approximation to what the low-energy part of this Hamiltonian looks like – the "low-energy effective Hamiltonian":

$$H = \Delta H_0 + H_1 \quad , \quad \|H_1\| \ll \Delta$$

$$H_{eff} \overset{\varepsilon,\eta}{\approx} H\big|_{\leq \Delta}$$

In our language H $(\Delta, \varepsilon, \eta)$–simunates H_{eff}.

Note: might look more familiar if we write this as

$$H' = H_0 + \varepsilon H_1$$

$$\|H_0\| = \|H_1\| = O(1), \qquad \varepsilon \ll 1.$$

Defining $\varepsilon = \frac{1}{\Delta}$ and rescaling, this is the same thing up to rescaling:

$$H' = \frac{H}{\Delta} = H_0 + \varepsilon H_1$$

However, more natural (and conventional) to take $\Delta \to \infty$ rather than $\varepsilon \to 0$ in quantum info. applications.

If H_0, H_1 do not commute, H_{eff} can look very different to either H_0 or V. So this provides a means of constructing non-trivial simulations:

Certain "gadgets" constructed in this way can be used to e.g. reduce k-body Hamiltonians to 2-body, or change the symmetry group of the local interactions, or put the local interactions on a planar graph, all whilst rigorously ensuring the entire physics (and hence also all properties such as the complexity class – see later) of the original Hamiltonian is approximately preserved.

We will develop perturbation theory in the Schrieffer-Wolff formalism, which is more powerful & better suited to proving full simulation than textbook formulations such as the Feynman-Dyson approach. (However, most of the applications and examples in this course could also be analysed via the Dyson resolvent / self-energy approach, and it's worth learning both!)

(For this section of the course, see [BDL'11] which gives a nice, self-contained development of this theory in quantum info language.)

Schrieffer-Wolff perturbation theory

General idea:

$\mathcal{H} = \mathcal{H}_- \oplus \mathcal{H}_+$,

$$H_0 = \begin{array}{cc} \left(\begin{array}{c|c} 0 & 0 \\ \hline 0 & H > \Delta \mathbb{1} \end{array}\right) & \begin{array}{c} \mathcal{H}_- \\ \mathcal{H}_+ \end{array} \end{array}$$

$H = \Delta H_0 + H_1$

$\|H_1\| < \frac{\Delta}{2}$

Find $U = e^S$, $S^\dagger = -S^\dagger$ that block-diagonalises H:

$$e^S H e^{-S} = \begin{array}{cc} \left(\begin{array}{c|c} H_{eff} & 0 \\ \hline 0 & H_{junk} \end{array}\right) & \begin{array}{c} \mathcal{H}_- \\ \mathcal{H}_+ \end{array} \end{array}$$

$$S = \begin{array}{cc} \left(\begin{array}{c|c} 0 & X \\ \hline -X^\dagger & 0 \end{array}\right) & \begin{array}{c} \mathcal{H}_- \\ \mathcal{H}_+ \end{array} \end{array}$$

Then "low energy" effective Hamiltonian is

$$H_{eff} = e^S H e^{-S}\big|_{\mathcal{H}_-}$$

Turns out there is a unique such S: called the "Schrieffer-Wolff" transform.

Express e^S as Taylor series in powers of H_1 $\longrightarrow$ rigorous perturbative expansion of H_{eff}, with analytic convergence bounds etc.

Direct rotation

Pair of states

$|\psi\rangle, |\phi\rangle \in \mathcal{H}$

Reflections $Z_\psi := \mathbb{1} - 2|\psi\rangle\langle\psi|$

$Z_\phi := \mathbb{1} - 2|\phi\rangle\langle\phi|$

Easy to check $Z_\phi Z_\psi$ rotates in 2-dimensional subspace $\mathrm{span}\{|\psi\rangle, |\phi\rangle\}$ by angle 2θ where $\theta = \cos^{-1}\langle\psi|\phi\rangle$ is angle between $|\psi\rangle$ & $|\phi\rangle$.

Cf. Grover algorithm.

Def.

Direct rotation $U_{\psi\to\phi} := \sqrt{Z_\phi Z_\psi}$

where $\sqrt{z}$ defined with branch cut along $-\mathbb{R}$ axis, $\sqrt{1} = 1$.

Well defined as long as $Z_\phi Z_\psi$ has no eigvals on branch cut.

Lemma

$|\psi\rangle, |\phi\rangle \in \mathcal{H}$ non-orthogonal : $\langle\psi|\phi\rangle \neq 0$.
Wlog choose global phase s.t $\langle\psi|\phi\rangle \in \mathbb{R}_+$.
Then

$$U_{\psi\to\phi} |\psi\rangle = |\phi\rangle.$$

Pf.

Since $U_{\psi\to\phi}$ rotates in 2dim subspace $R = \text{span}\{|\psi\rangle, |\phi\rangle\}$ & leaves $R^\perp$ invariant, suffices to restrict to $R \equiv \mathbb{C}^2$.

Wlog denote
$|\psi\rangle = |1\rangle, \quad |\phi\rangle = \sin\theta\,|0\rangle + \cos\theta\,|1\rangle,$
where $0 \leq \theta < \frac{\pi}{2}$ by assumption.

From Def:

$$Z_\psi = \sigma_z, \qquad Z_\phi = \cos 2\theta\,\sigma_z - \sin 2\theta\,\sigma_x$$

Exercise: Show $Z_\phi Z_\psi = e^{i 2\theta \sigma_y}$

(straightforward calculation)

$0 \leq 2\theta < \pi \Rightarrow$ no eigval on $-\mathbb{R}$

$\Rightarrow U_{\psi\to\phi} = \sqrt{Z_\phi Z_\psi} = e^{i\theta\sigma_y}$ uniquely defined.

Exercise: Show $U_{\psi\to\phi}|1\rangle = \sin\theta\,|0\rangle + \cos\theta\,|1\rangle$
$= |\phi\rangle$

(straightforward calculation) $\square$

Corollary

$|\psi\rangle, |\phi\rangle \in \mathcal{H}$ non-orthogonal

$P := |\psi\rangle\langle\psi|, \quad P_0 := |\phi\rangle\langle\phi|.$

Direct rotation

$$U_{\psi\to\phi} = e^{S}$$

where S is anti-Hermitian ($S^\dagger = -S$) and satisfies

- $$PSP = P_0 S P_0 = (\mathbb{1}-P)S(\mathbb{1}-P) = (\mathbb{1}-P_0)S(\mathbb{1}-P_0) = 0$$
- $\|S\| < \frac{\pi}{2}$

Moreover this S is uniquely defined.

Simultaneously block off-diagonal wrt. $|\psi\rangle$ <u>and</u> $|\phi\rangle$:

$$S = \begin{array}{c} \left(\begin{array}{c|c} 0 & A \\ \hline -A^\dagger & 0 \end{array}\right) \end{array} \begin{array}{l} |\psi\rangle \\ |\psi\rangle^\perp \end{array} = \left(\begin{array}{c|c} 0 & B \\ \hline -B^\dagger & 0 \end{array}\right) \begin{array}{l} |\phi\rangle \\ |\phi\rangle^\perp \end{array}$$

<u>Pf.</u> Exercise: straightfoward algebra.

Pair of subspaces

Subspaces $\mathcal{P}, \mathcal{P}_0 \subseteq \mathcal{H}$,
P, P_0 projectors onto these.

Lemma

$$\| P - P_0 \| < 1$$
$$\Leftrightarrow$$
$$\forall\, |\psi\rangle \in \mathcal{P},\ |\phi\rangle \in \mathcal{P}_0 :\quad \langle \psi | \phi \rangle \neq 0$$

Pf. Exercise

Reflections
$$Z_{\mathcal{P}} := 2P - \mathbb{1}$$
$$Z_{\mathcal{P}_0} := 2P_0 - \mathbb{1}$$

Def.
Direct rotation from $\mathcal{P}$ to $\mathcal{P}_0$

$$U_{\mathcal{P}\to\mathcal{P}_0} := \sqrt{Z_{\mathcal{P}_0} Z_{\mathcal{P}}}$$

($\sqrt{z}$ as before)

Lemma

$\| P - P_0 \| < 1$.
U uniquely defined by Def.
$U P U^{\dagger} = P_0$

To prove this, we need a result known in the quantum info. community as Jordan's Lemma (which has myriad uses across many areas of the field, so is well worth knowing in its own right!)

<u>Lemma</u> (Jordan)

Projectors P, P_0

$\exists\, U$ s.t. $U P_0 U^\dagger = \bigoplus_i D_i$ diagonal

$U P U^\dagger = \bigoplus_i P_i$ block-diagonal

where each D_i, P_i is 1×1 or 2×2

rank $D_i \leq 1$

rank $P_i \leq 1$.

$$U P_0 U^\dagger = \begin{pmatrix} 1 & & & & & & \\ & 1 & & & & & \\ & & 1 & & & & \\ & & & \ddots & & & \\ & & & & 0 & & \\ & & & & & 0 & \\ & & & & & & \ddots \\ & & & & & & & 0 \end{pmatrix}$$

$$U P U^\dagger = \begin{pmatrix} \boxed{1} & & & & & \\ & \boxed{0} & & & & \\ & & \boxed{P_3} & & & \\ & & & \boxed{1} & & \\ & & & & \boxed{P_4} & \\ & & & & & \ddots \end{pmatrix}$$

Pf. (of direct rotation Lemma)

Jordan's Lemma
$\Rightarrow$ P, P_0 hence also Z_P, Z_{P_0}, $U_{P\to P_0}$ simultaneously block-diagonalisable

Suffices to prove Lemma for P, P_0 1×1 or 2×2 matrices.

1×1:
$\|P-P_0\| < 1 \Rightarrow P = P_0 = 0$ or $1 \Rightarrow U=1$
Lemma holds trivially.

2×2:
rank 1 $\Rightarrow$ $P = |\psi\rangle\langle\psi|$, $P_0 = |\phi\rangle\langle\phi|$
$\|P-P_0\| < 1 \Rightarrow \langle\psi|\phi\rangle \neq 0$

This is the special case of a pair of states, which we already proved above. $\square$

Corollary
$U_{P\to P_0} = e^S$, $S = -S^\dagger$ satisfying

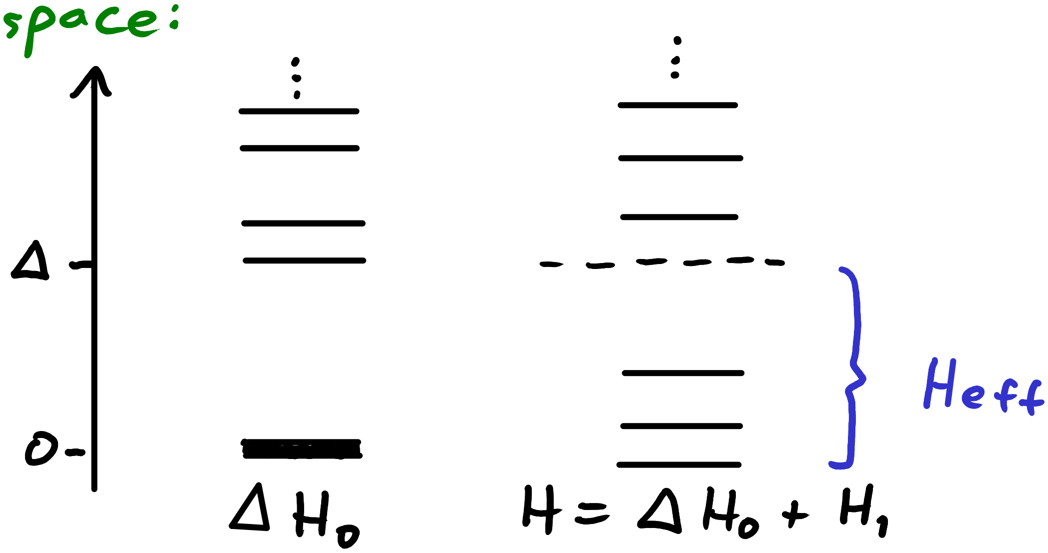
- $PSP = P_0 S P = (\mathbb{1}-P)S(\mathbb{1}-P) = (\mathbb{1}-P_0)S(\mathbb{1}-P_0) = 0$

  Simultaneously block-off-diagonal wrt $P, P^\perp$ & $P_0, P_0^\perp$
- $\|S\| < \frac{\pi}{2}$

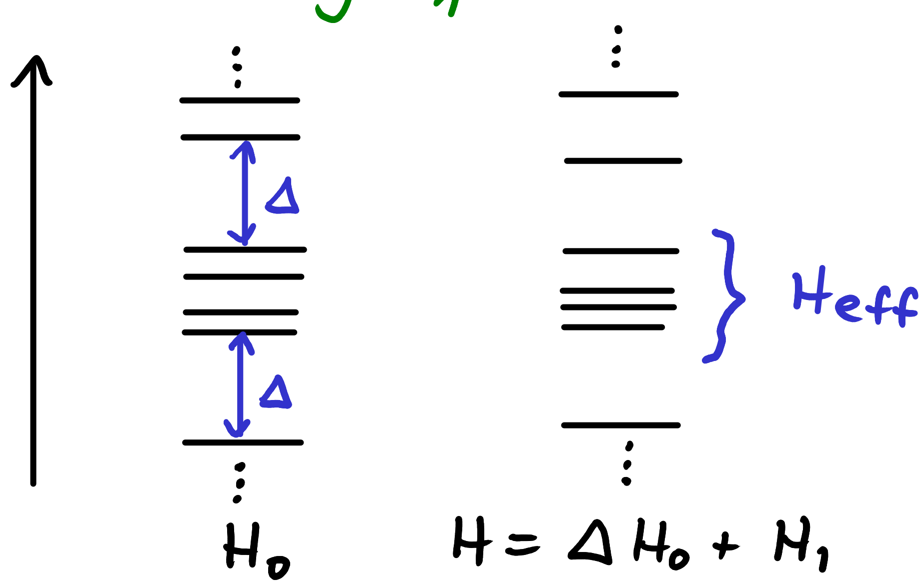
Pf. Apply pair-of-states corollary to each block.

Effective Hamiltonian

Note we will state all results for effective Hamiltonians on the "low-energy" subspace (i.e. energy below some cut-off, which could however be large). We will also restrict to the case where the unperturbed Hamiltonian has energy $=0$ on this subspace:



However, the results generalise straightforwardly to <u>any</u> spectrally separated eigenspace



Def. (Schrieffer – Wolff transformation)

$\mathcal{H} = \mathcal{H}_- \oplus \mathcal{H}_+$

$P_\pm :=$ orthogonal projectors onto $\mathcal{H}_\pm$

$$H = \Delta H_0 + H_1$$

$$H_0 = \left(\begin{array}{c|c} 0 & 0 \\ \hline 0 & \geq \mathbb{1} \end{array}\right)\begin{array}{l} \mathcal{H}_- \\ \mathcal{H}_+ \end{array}, \qquad \|V\| < \frac{\Delta}{2}$$

$\mathcal{P}_0 := \mathcal{H}_-$

$\mathcal{P} := \operatorname{span}\{ |\psi\rangle : H|\psi\rangle = \lambda|\psi\rangle,\ \lambda \leq \Delta \}$

Direct rotation $U_{\mathcal{P}\to\mathcal{P}_0}$ is called the "Schrieffer – Wolff transformation" for ΔH_0, H_1 wrt. $\mathcal{P}_0$.

$$H_{eff} = P_- e^S H e^S P_-$$

Note: e^S unitary so

$$\operatorname{spec} H_{eff}\big|_{\mathcal{H}_-} = \operatorname{spec} H\big|_{\mathcal{H}_-}$$

Notation: $A_{--} := P_- A P_-$, $A_{++} := P_+ A P_+$

$A_{-+} := P_- A P_+$, $A_{+-} := P_+ A P_-$

So far, this isn't very useful in practice. We have shown there <u>exists</u> a SW transformation S with certain properties. But this doesn't give us a method of <u>constructing</u> S from H_0, H_1.

Indeed, there always exists <u>some</u> unitary that transforms from the eigenbasis of H_0 to the eigenbasis of H. The key is that the additional properties of the SW transform (block-off-diagonal etc.) allow us to find convergent series expansions for S & H_{eff} in terms of H_0, H_1.

<u>Lemma</u>

S satisfies

$$\tanh(\hat{S})(H_0 + \varepsilon H_{diag}) + \varepsilon H_{off\text{-}diag} = 0 \quad (*)$$

where
$$H_{diag} = P_- H_1 P_- + P_+ H_1 P_+$$
$$H_{off\text{-}diag} = P_- H_1 P_+ + P_+ H_1 P_-$$
$$e^{\hat{S}}(M) = e^S M e^{-S}$$

<u>Pf.</u>

Start from block-structure of S & $e^S H e^{-S}$ & do algebra (see [BDL'11], Sec. 3.2)

Thm.

$$S = \sum_{k=1}^{\infty} S_j \,, \qquad \| S_j \| = O(\Delta^{-j} \| H_1 \|)$$

$$\| S \| = O(\Delta^{-1} \| H_1 \|)$$

$$H_{eff} = (e^{S} H e^{-S})_{--} = \sum_{j=1}^{\infty} H_{eff,j}$$

$$\| H_{eff,j} \| = O\left(\frac{1}{\Delta^j}\right)$$

$$\| H_{eff} - \sum_{j=1}^{k} H_{eff,j} \| = O(\Delta^{-k} \| H_1 \|^{k+1})$$

In particular,

$$H_{eff,1} = P_- H_1 P_- =: (H_1)_{--}$$

$$H_{eff,2} = -\Delta^{-1} (H_1)_{-+} H_0^{-1} (H_1)_{+-}$$

Note: $P_+ H_0 P_+ \geq \mathbb{1}$ by assumption, so $P_+ H_0^{-1} P_+ = (P_+ H_0 P_+)^{-1}$ in 2nd order term is well-defined.

Pf.

Taylor-expand $\tanh(\hat{S})$ & solve order by order (see [BDL '11], Sec. 3.2).

There is a systematic diagrammatic procedure for constructing $H_{eff,j}$ recursively, analogous (but different) to Feynman diagrams arising from Feynman-Dyson perturbation theory. (See [BDL '11], Sec. 3.3.)

However, for everything we do here, we will only need to go up to 2nd order, given above. And almost nothing in the quantum info. literature requires going beyond 3rd order. (I'm aware of just one result that requires 4th order.)

Perturbation Gadgets

We will use this to derive a systematic way of constructing "gadgets" that allow us to transform an initial many-body Hamiltonian into a simpler one (in some sense) that $(\Delta, \varepsilon, \eta)$-simulates it, following [OT '08].

Lemma (1st order simulation)

Target Hamiltonian H_{target} on $\mathcal{H}'$
Hamiltonians H_0, H_1 on $\mathcal{H} = \mathcal{H}_- \oplus \mathcal{H}_+$

If $\exists$ local encoding $\mathcal{E}$ with isometry V & encoding $\tilde{\mathcal{E}}$ with isometry $\tilde{V} : \mathcal{H}' \to \mathcal{H}_-$ s.t. $\|\tilde{V} - V\| \leq \eta$, and if

$$\| \tilde{\mathcal{E}}(H_{target}) - (H_1)_{--} \| \leq \frac{\epsilon}{2}, \text{ then}$$

for $\Delta \geq O\left(\|H_1\|^2 / 2\epsilon + \|H_1\| / \eta \right)$

$H_{sim} = \Delta H_0 + H_1$ $\quad (\frac{\Delta}{2}, \epsilon, \eta)$-simulates H_{target}.

Pf.

Let $\tilde{\mathcal{E}}(H_{target}) = e^{S} \mathcal{E}(H_{target}) e^{-S}$.
so associated isometry is $\tilde{V} = e^{S} V$

Need to show $\tilde{\mathcal{E}}$ satisfies properties (i) & (ii) of simulation Def.

(i):

- By Def, SW tranform maps $\mathcal{H}_-$ to low-energy subspace of H_{sim}, so $\tilde{\mathcal{E}}(\mathbb{1})$ = projector onto low-energy eigspace
- $$\|\tilde{V} - V\| = \|e^{S} V - V\| \leq \|e^{S} - \mathbb{1}\|$$
$$\leq \|S\|$$
$$= O(\Delta^{-1} \|H_1\|) \quad \text{by Thm.}$$
$$\leq \eta \quad \text{by assumption}$$

(ii):

$$\|H_{sim}|_{\leq \Delta} - \tilde{\mathcal{E}}(H_{target})\|$$
$$\leq \|H_{sim}|_{\leq\Delta} - (H_1)_{--}\| + \|(H_1)_{--} - \tilde{\mathcal{E}}(H_{target})\| \quad \text{triangle ineq}$$
$$\leq O(\Delta^{-1} \|H_1\|^2) + \frac{\epsilon}{2} \quad \text{by SW + conditions in Lemma}$$
$$\leq \frac{\epsilon}{2} + \frac{\epsilon}{2} = \epsilon. \quad \text{by conditions in Lemma}$$

$\square$

Lemma (2nd order simulation)

Target Hamiltonian H_{target} on $\mathcal{H}'$.

Hamiltonians H_0, H_1, H_2 on $\mathcal{H} = \mathcal{H}_- \oplus \mathcal{H}_+$
s.t. H_1 block-diagonal, $(H_2)_{--} = 0$.

If $\exists$ local encoding $\mathcal{E}$ with isometry V
& encoding $\tilde{\mathcal{E}}$ with isometry $\tilde{V} : \mathcal{H}' \to \mathcal{H}_-$
s.t. $\| \tilde{V} - V \| \leq \eta$, and if

$$\| \mathcal{E}(H_{target}) - (H_1)_{--} - (H_2)_{-+} H_0^{-1} (H_2)_{+-} \| \leq \frac{\varepsilon}{2}$$

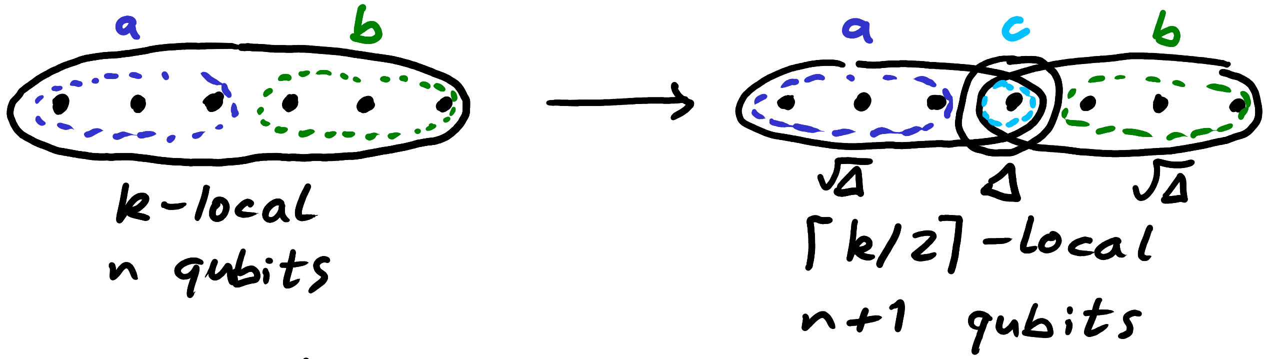
then for $\Delta \geq O\left(\frac{\Lambda^6}{2\varepsilon^3} + \frac{\Lambda^3}{\eta^3}\right)$, $\Lambda := \max(\|H_1\|, \|H_2\|)$

$$H_{sim} = \Delta H_0 + \sqrt{\Delta} H_1 + H_2$$

is a $(\frac{\Delta}{2}, \varepsilon, \eta)$-simulation of H_{target}.

Pf. Similar to 1st order.

Example: subdivision gadget [OT'08]



$$H_{target} = A_a B_b$$

Let $H_0 = |1\rangle\langle 1|_c$, $\quad H_1 = \frac{1}{2}(A_a^2 + B_b^2)$

$$H_2 = \frac{1}{\sqrt{2}}(A_a X_c - X_c B_b) \qquad \text{(Pauli } X\text{)}$$

$$(H_2)_{-+} = \frac{1}{\sqrt{2}} |0\rangle\langle 1|_c (A_a - B_b)$$

$$(H_2)_{-+} H_0^{-1} (H_2)_{+-} = \frac{1}{2} |0\rangle\langle 0|_c (A_a - B_b)^2$$

$$= |0\rangle\langle 0|_c \left(\frac{1}{2}A_a^2 - A_a B_b + \frac{1}{2} B_b^2\right)$$

$$(H_1)_{--} = \frac{1}{2} |0\rangle\langle 0|_c (A_a^2 + B_b)^2$$

Let $V|\psi\rangle_{ab} = |\psi\rangle_{ab}|0\rangle_c$. Then

$$(H_1)_{--} - (H_2)_{-+} H_0^{-1} (H_2)_{+-} = V H_{target} V^\dagger .$$

Fulfils conditions of Lemma, so

$H_{sim} = \Delta H_0 + \sqrt{\Delta} H_2 + H_1 \quad (\Delta/2, \varepsilon, \eta)$-simulates H_{target}.

Note H_{sim} only contains interactions on at most $\max(|a|+1, |b|+1)$ qudits, so have reduced locality from $k \rightarrow \lceil k/2 \rceil + 1$.