1 Spectral properties

Lemma 1 (moments).

$$\frac{1}{d}\sum_j E_j^m = \langle H^m \rangle = \Theta(n^{m/2}), \quad \forall \text{ even positive integer } m, \tag{1}$$

$$\left|\frac{1}{d}\sum_j E_j^3\right| = |\langle H^3 \rangle| = O(n). \tag{2}$$

Proof. Expanding H in the Pauli basis, it suffices to count the number of terms that do not vanish upon taking the trace in the expansion of H^m or H^3. □

Lemma 2 (concentration of eigenvalues). *Almost all eigenstates have zero energy density:*

$$|\{j : |E_j| \ge n^{0.51}\}|/d \le O(n^{-0.01m}), \quad \forall m > 0. \tag{3}$$

Proof. It follows from Eq. (1) and Markov's inequality. □

This lemma allows us to upper bound the total contribution of all eigenstates away from the middle of the spectrum, e.g.,

$$\frac{1}{d}\sum_{j:|E_j|\ge n^{0.51}} E_j^2 \le O(n^{2-0.01m}), \quad \forall m > 0. \tag{4}$$

2 Eigenstate thermalization

It suffices to assume ETH for eigenstates in the middle of the spectrum.

Assumption 1 (eigenstate thermalization hypothesis in the middle of the spectrum). Let δ be an arbitrarily small positive constant. For any local operator X with $\|X\| \le 1$, there is a function $f_X : [-\delta, \delta] \to [-1, 1]$ such that

$$|X_{jj} - f_X(E_j/n)| \le 1/\operatorname{poly} n \tag{5}$$

for all j with $|E_j| \le \delta n$, where $\operatorname{poly} n$ denotes a polynomial of sufficiently high degree in n. We assume that f_X is smooth in the sense of having a Taylor expansion to some low order.

Lemma 3. *For any local operator X and traceless local operator A, Assumption 1 implies*

$$f_X(0) = \frac{1}{d}\operatorname{tr} X, \tag{6}$$

$$f'_A(0) = \operatorname{tr}(HA)/\operatorname{tr}(HH_i), \tag{7}$$

$$\frac{1}{d}\sum_j |A_{jj}|^2 = \frac{|\operatorname{tr}(HA)|^2}{dn\operatorname{tr}(HH_i)} + O(n^{-2}), \tag{8}$$

$$\frac{1}{d}\sum_j |A_{jj}|^4 = O(n^{-2}). \tag{9}$$

For a generic traceless local operator A, the right-hand side of Eq. (7) (the normalized overlap between A and the Hamiltonian) is finite and the first term on the right-hand side of Eq. (8) is $\Theta(1/n)$.

Proof of Eq. (6).

$$\frac{1}{d}\operatorname{tr}X=\frac{1}{d}\sum_j X_{jj}\approx\frac{1}{d}\sum_{j:|E_j|<n^{0.51}}X_{jj}\approx\frac{1}{d}\sum_{j:|E_j|<n^{0.51}}f_X(0)\approx\frac{1}{d}\sum_j f_X(0)=f_X(0), \tag{10}$$

where we used Lemma 2 in the second and fourth steps. The third step follows from the continuity of $f_X(x)$ at $x=0$. Taking the limit $n\to\infty$, all errors in Eq. (10) vanish and thus we obtain Eq. (6). In particular, $f_A(0)=0$ for any traceless local operator A. □

Proof of Eq. (7).

$$\begin{aligned}\frac{1}{d}\operatorname{tr}(HA)=\frac{1}{d}\sum_j E_jA_{jj}\approx\frac{1}{d}\sum_{j:|E_j|<n^{0.51}}E_jA_{jj}\approx\frac{1}{d}\sum_{j:|E_j|<n^{0.51}}\frac{E_j^2}{n}f_A'(0)\approx\frac{1}{d}\sum_j\frac{E_j^2}{n}f_A'(0)\\ =\operatorname{tr}(HH_i)f_A'(0)/d,\end{aligned} \tag{11}$$

where we used Lemma 2 and Eq. (4) in the second and fourth steps, respectively. In the third step, we used Eq. (5) and the Taylor expansion

$$f_A(E_j/n)=f_A(0)+f_A'(0)E_j/n+0.5f_A''(0)E_j^2/n^2+O(|E_j|^3/n^3) \tag{12}$$

so that the approximation error in this step is upper bounded by

$$\frac{O(1)}{d}\sum_{j:|E_j|<n^{0.51}}\frac{|E_j|^3}{n^2}\le O(n^{-0.47}). \tag{13}$$

Taking the limit $n\to\infty$, all errors in Eq. (11) vanish and thus we obtain Eq. (7). □

Proof of Eq. (8).

$$\frac{1}{d}\sum_j|A_{jj}|^2\approx\frac{1}{d}\sum_{j:|E_j|<n^{0.51}}|A_{jj}|^2\approx\frac{|f_A'(0)|^2}{d}\sum_{j:|E_j|<n^{0.51}}\frac{E_j^2}{n^2}\approx\frac{|f_A'(0)|^2}{d}\sum_j\frac{E_j^2}{n^2}=\frac{|\operatorname{tr}(HA)|^2}{dn\operatorname{tr}(HH_i)}, \tag{14}$$

where we used Lemma 2 and Eqs. (4), (7) in the first, third, and last steps, respectively. In the second step, we used Eqs. (5), (12) with the approximation error upper bounded by

$$\begin{aligned}\frac{O(1)}{d}\left|\sum_{j:|E_j|<n^{0.51}}\frac{E_j^3}{n^3}\right|+\frac{O(1)}{d}\sum_{j:|E_j|<n^{0.51}}\frac{E_j^4}{n^4}+1/\operatorname{poly}n\approx\frac{O(1)}{d}\left|\sum_j\frac{E_j^3}{n^3}\right|+\frac{O(1)}{d}\sum_j\frac{E_j^4}{n^4}\\ =O(n^{-2})+O(n^{-2})=O(n^{-2}),\end{aligned} \tag{15}$$

where we used Eqs. (1), (2). □

Proof of Eq. (9).

$$\frac{1}{d}\sum_j|A_{jj}|^4\approx\frac{1}{d}\sum_{j:|E_j|<n^{0.51}}|A_{jj}|^4\approx\frac{O(1)}{d}\sum_{j:|E_j|<n^{0.51}}\frac{E_j^4}{n^4}\approx\frac{O(1)}{d}\sum_j\frac{E_j^4}{n^4}=O(n^{-2}). \tag{16}$$

□

3 Error analysis for Eq. (6) in the main text

Let c be a sufficiently large constant. Consider the first term on the right-hand side of Eq. (10) in the main text:

$$\frac{1}{d}\sum_{j,k} A_{jj}B_{jk}C_{kk}D_{kj} \approx \frac{1}{d}\sum_{j}\sum_{k:|E_j-E_k|<c\ln n} A_{jj}B_{jk}C_{kk}D_{kj} \approx \frac{1}{d}\sum_{j}\sum_{k:|E_j-E_k|<c\ln n} A_{jj}B_{jk}C_{jj}D_{kj}$$
$$\approx \frac{1}{d}\sum_{j,k} A_{jj}C_{jj}B_{jk}D_{kj} = \frac{1}{d}\sum_{j} A_{jj}C_{jj}(BD)_{jj}. \quad (17)$$

In the first and third steps, we used Lemma 2 in the main text: Due to the presence of off-diagonal matrix elements B_{jk}, D_{kj}, the total contribution of all terms with $|E_j-E_k| \geq c\ln n$ is upper bounded by $1/\operatorname{poly} n$. In the second step of Eq. (17), we replace C_{kk} by C_{jj} using ETH (Assumption 1), which states that eigenstates with similar energies have similar local expectation values. A detailed and rigorous error analysis for Eq. (17) is given below.

Proposition 1. *The approximation errors in the first and third steps of Eq. (17) are* $1/\operatorname{poly} n$*, where* $\operatorname{poly} n$ *denotes a polynomial of sufficiently high degree in* n*.*

Proof. Let

$$Q_j = \sum_{k:|E_j-E_k|\geq c\ln n} |k\rangle\langle k|, \quad \tilde{C} = \sum_k C_{kk}|k\rangle\langle k|. \quad (18)$$

Since $\tilde{C}$ is the diagonal part of C (in the energy eigenbasis), it is easy to see $\|\tilde{C}\| \leq \|C\|$. The approximation error in the first step of Eq. (17) is

$$\frac{1}{d}\left|\sum_j \sum_{k:|E_j-E_k|\geq c\ln n} A_{jj}B_{jk}C_{kk}D_{kj}\right| \leq \frac{1}{d}\sum_j |A_{jj}| \left|\sum_{k:|E_j-E_k|\geq c\ln n} B_{jk}C_{kk}D_{kj}\right|$$
$$\leq \frac{\|A\|}{d}\sum_j |\langle j|BQ_j\tilde{C}Q_jD|j\rangle| \leq \frac{\|A\|}{d}\sum_j \|Q_jB^\dagger|j\rangle\|\|\tilde{C}\|\|Q_jD|j\rangle\| \leq \|A\|\|B\|\|C\|\|D\|/\operatorname{poly} n,$$
$$(19)$$

where we used Lemma 2 in the main text. The approximation error in the third step of Eq. (17) can be upper bounded similarly. □

Proposition 2. *The approximation error in the second step of Eq. (17) is* $\tilde{O}(n^{-1.5})$*.*

Proof. Let n be sufficiently large such that $n^{0.51} + c\ln n < \delta n$, and define

$$\tilde{C}^{(j)} := \sum_{k:|E_j-E_k|<c\ln n} (C_{jj} - C_{kk})|k\rangle\langle k|. \quad (20)$$

For j, k such that $|E_j| < n^{0.51}$ and $|E_j - E_k| < c\ln n$, Assumption 1 implies

$$|C_{jj} - C_{kk}| \leq |f_C(E_j/n) - f_C(E_k/n)| + 1/\operatorname{poly} n = O(|E_j - E_k|)/n + 1/\operatorname{poly} n. \quad (21)$$

Hence, $\|\tilde{C}^{(j)}\| = \tilde{O}(1/n)$ for any j such that $|E_j| < n^{0.51}$. The approximation error in the second step of Eq. (17) is

$$\begin{aligned}
&\frac{1}{d}\left|\sum_j \sum_{k:|E_j-E_k|<c\ln n} A_{jj}B_{jk}(C_{jj}-C_{kk})D_{kj}\right| \le \frac{1}{d}\sum_j |A_{jj}|\left|\sum_{k:|E_j-E_k|<c\ln n} B_{jk}\tilde{C}^{(j)}_{kk}D_{kj}\right| \\
&= \frac{1}{d}\sum_j |A_{jj}||\langle j|B\tilde{C}^{(j)}D|j\rangle| \le \frac{1}{d}\sum_j |A_{jj}|\left\|\tilde{C}^{(j)}\right\| \\
&= \frac{1}{d}\sum_{j:|E_j|<n^{0.51}} |A_{jj}|\left\|\tilde{C}^{(j)}\right\| + \frac{1}{d}\sum_{j:|E_j|\ge n^{0.51}} |A_{jj}|\left\|\tilde{C}^{(j)}\right\| \\
&\le \frac{1}{d}\sum_{j:|E_j|<n^{0.51}} |A_{jj}|\tilde{O}(1/n) + \frac{1}{d}\sum_{j:|E_j|\ge n^{0.51}} |A_{jj}|O(1) \le \frac{\tilde{O}(1/n)}{d}\sum_j |A_{jj}| + \frac{1}{d}\sum_{j:|E_j|\ge n^{0.51}} O(1) \\
&\le \tilde{O}(1/n)\sqrt{\frac{1}{d}\sum_j |A_{jj}|^2} + 1/\operatorname{poly} n = \tilde{O}(n^{-1.5}),
\end{aligned} \tag{22}$$

where we used Eq. (8) in the last step. □

4 Error analysis for Eq. (7) in the main text

The third term on the right-hand side of Eq. (19) in the main text is

$$\frac{1}{d}\sum_j |A_{jj}B_{jj}|^2 \le \frac{1}{2d}\sum_j |A_{jj}|^4 + |B_{jj}|^4 = O(n^{-2}), \tag{23}$$

where we used Eq. (9). A rigorous error analysis for Eq. (20) in the main text is given below.

Proposition 3. *The error in Eq. (20) in the main text is $O(n^{-2})$.*

Proof. The approximation error in the last step of Eq. (20) in the main text is $O(n^{-2})$ as given by Eq. (8). Using the Taylor expansion of $f_{AA^\dagger}(x)$ at $x = 0$, we estimate the approximation error in the second step of Eq. (20) in the main text:

$$\begin{aligned}
&\frac{O(1)}{d}\left|\sum_{j:|E_j|<n^{0.51}} \frac{|B_{jj}|^2E_j}{n}\right| + \frac{O(1)}{d}\sum_{j:|E_j|<n^{0.51}} \frac{|B_{jj}|^2E_j^2}{n^2} + 1/\operatorname{poly} n \\
&\lesssim \frac{O(1)}{d}\left|\sum_{j:|E_j|<n^{0.51}} \frac{E_j^3}{n^3}\right| + \frac{O(1)}{d}\sum_{j:|E_j|<n^{0.51}} \left(\frac{E_j^4}{n^4} + |B_{jj}|^4\right) \\
&\approx \frac{O(1)}{d}\left|\sum_j \frac{E_j^3}{n^3}\right| + \frac{O(1)}{d}\sum_j \left(\frac{E_j^4}{n^4} + |B_{jj}|^4\right) \approx O(n^{-2}) + O(n^{-2}) + O(n^{-2}) = O(n^{-2}),
\end{aligned} \tag{24}$$

where we used the Taylor expansion of $f_B(x)$ at $x = 0$ and the inequality of arithmetic and geometric means in the first step; Lemma 2 in the second step; Eqs. (1), (2), (9) in the third step. □