AKLT models on decorated square lattices are gapped

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Abdul-Rahman et al. in \textsuperscript{[1]} provided an elegant approach and proved analytically the existence of nonzero spectral gap for the AKLT models on the decorated honeycomb lattice (for the number $n$ of spin-1 decorated sites on each original edge to be no less than 3). We perform the same calculations for the decorated square lattice and show that the corresponding AKLT models are gapped if $n \geq 4$. Furthermore, using the results from both the decorated honeycomb and square lattice, we also show analytically that a family of decorated hybrid AKLT models, whose original lattice is of mixed vertex degrees 3 and 4, are also gapped for $n \geq 4$. Our numerical results further improve the nonzero gap to $n \geq 2$.

I. INTRODUCTION

Affleck, Kenedy, Lieb, and Tasaki (AKLT) constructed a one-dimensional spin-1 spin chain whose Hamiltonian is rotation-invariant in the spin degree of freedom \textsuperscript{[2]}, but has a spectral gap above the unique ground state, in contrast to the spin-1/2 antiferromagnetic Heisenberg model. This provided a strong support for Haldane’s conjecture \textsuperscript{[3,4]} regarding the spectral gap and the spin magnitudes. They also generalized the construction to two dimensions \textsuperscript{[5]}. They showed that the spin-spin correlation function of the ground-state wavefunction decays exponentially in the honeycomb and the square lattice models. The uniqueness of the ground state in these models was further analyzed by Kenedy, Lieb and Tasaki \textsuperscript{[6]}. There have been a few useful techniques for showing uniqueness of the ground state and gap \textsuperscript{[6,8]}, but the proof of the nonzero spectral gap has not been established for either of the two 2D AKLT models, even after more than three decades of their construction.

Unexpectedly, 2D AKLT states have recently emerged as resource for universal quantum computation (via local measurement), in the framework of the measurement-based quantum computation (MBQC) \textsuperscript{[9–12]}. The spin-3/2 AKLT state on the honeycomb lattice was first shown to provide the appropriate entanglement structure for universal QC \textsuperscript{[13–14]}, a result subsequently generalized to other trivalent lattices \textsuperscript{[15]}. In order to demonstrate the computation universality for the spin-2 AKLT state on the square lattice \textsuperscript{[16]}, a few decorated lattice structures (with mixed vertex degrees) and the corresponding AKLT states were first considered and shown to be universal in Ref. \textsuperscript{[17]}. Regarding the gap, tensor network methods were employed and the value of the gap in the thermodynamic limit was estimated \textsuperscript{[19,20]}. A recent breakthrough from the analytic perspective was given by Abdul-Rahman et al. \textsuperscript{[1]}, who considered a family of decorated honeycomb lattices and proved that the corresponding AKLT models are gapped for the number $n$ of decorated site being greater than 2 (see e.g. Fig. \textsuperscript{[1]a}). The AKLT states, according to the results in Ref. \textsuperscript{[17]}, are also universal for MBQC, and hence are also of practical interest. Additional progress has also been made by Lemm, Sandvik and Yang on hexagonal chains \textsuperscript{[21]}, where the quasi-1D AKLT models are also gapped.

We note that the results of Ref. \textsuperscript{[1]} seem to apply straightforwardly to other trivalent lattices with deco-
model Hamiltonian defined on denotes the edge set of the decorated lattice. The AKLT original lattice may have some slight differences. Consider will try to follow the same symbols in Ref. [1] as much as possible, but may have some slight differences. Consider an original lattice (e.g. honeycomb or square lattice) and its decorated version \( \Lambda^{(n)} \) having each edge of the original lattice \( \Lambda \) decorated with \( n \) spin-1 sites. Let \( \mathcal{E}_{\Lambda^{(n)}} \) denotes the edge set of the decorated lattice. The AKLT model Hamiltonian defined on \( \Lambda^{(n)} \) is

\[
H_{\Lambda^{(n)}}^{\text{AKLT}} = \sum_{e \in \mathcal{E}_{\Lambda^{(n)}}} P_e^{(z(e)/2)},
\]

where \( P_e^{(z(e)/2)} \) is a projection to total spin \( s = z(e)/2 \) subspace of the two spins linked by the edge \( e \), and \( z(e) \) denotes the sum of the coordination numbers (i.e. vertex degrees) of the two spins.

Instead of directly using the AKLT Hamiltonian, one first considers a slightly modified one:

\[
H_Y \equiv \sum_{v \in \Lambda} h_v = \sum_{v \in \Lambda} \sum_{e \in \mathcal{E}_{Y_v}} P_e^{(z(e)/2)},
\]

where \( h_v \) is the AKLT Hamiltonian on the set \( Y_v \) of \( (zn + 1) \) vertices of the decorated lattice \( \Lambda^{(n)} \), \( z \) is the coordination number (\( z = 3 \) for the honeycomb) and \( \mathcal{E}_{Y_v} \) denotes the edges connecting vertices in \( Y_v \); see Fig. 2 for illustration. It has a few terms in \( H_{\Lambda^{(n)}}^{\text{AKLT}} \) missing, i.e., those terms on the edges containing the last spin-1 site on edge \( e \in Y_v \) and the next site \( v' \in \Lambda \). So we have an inequality

\[
H_{\Lambda^{(n)}}^{\text{AKLT}} \leq H_Y \leq 2H_{\Lambda^{(n)}}^{\text{AKLT}}.
\]

However, instead of \( H_Y \), we consider a slight modification

\[
\tilde{H}_{\Lambda^{(n)}} = \sum_{v \in \Lambda} P_v,
\]

where \( P_v \) is the orthogonal projection onto the range of \( h_v \). The kernel of \( P_v \) is the ground space of \( h_v \), i.e., \( \ker P_v = \ker h_v \). Then it is shown that

\[
\frac{\gamma_Y}{2} \tilde{H}_{\Lambda^{(n)}} \leq H_{\Lambda^{(n)}}^{\text{AKLT}} \leq ||h_v|| \tilde{H}_{\Lambda^{(n)}},
\]

where \( \gamma_Y \) is the smallest nonzero eigenvalue of \( h_v \) (or equivalently the spectral gap of the small system \( Y_v \)) and \( ||h_v|| \) is the usual operator norm of \( h_v \) (or equivalently the largest eigenvalue of \( h_v \), since \( h_v \) is non-negative). The strategy is to prove \( \tilde{H}_{\Lambda^{(n)}} \) is gapped. By squaring \( \tilde{H}_{\Lambda^{(n)}} \), we find that

\[
(\tilde{H}_{\Lambda^{(n)}})^2 = \tilde{H}_{\Lambda^{(n)}} + \sum_{v \neq w} (P_v P_w + P_w P_v) \geq \tilde{H}_{\Lambda^{(n)}} + \sum_{(v,w) \in \mathcal{E}_{\Lambda}} (P_v P_w + P_w P_v),
\]

where for those \( v \) and \( w \) not on the same edge \( P_v P_w \) is non-negative. If one can find the minimum positive number \( \chi_n > 0 \) such that \( P_v P_w + P_w P_v \geq -\chi_n (P_v + P_w) \), then

\[
(\tilde{H}_{\Lambda^{(n)}})^2 = \tilde{H}_{\Lambda^{(n)}} - \sum_{v \neq w} (P_v + P_w) \geq (1 - \chi_n/z) \tilde{H}_{\Lambda^{(n)}} = \gamma \tilde{H}_{\Lambda^{(n)}},
\]

where \( \gamma \equiv 1 - z \chi_n \) and \( z \) is the coordination number of the original lattice \( \Lambda \) (e.g. \( z = 3 \) for the honeycomb and \( z = 4 \) for the square lattice). If \( \gamma > 0 \), then one proves that \( \tilde{H}_{\Lambda^{(n)}} \) has a spectral gap above the ground state(s).

Therefore, most of effort goes into finding \( \chi \) or its upper bound. One that was used in Ref. [11] is the Lemma 6.3 from Ref. [7] for a pairs of projectors \( E \) and \( F \):

\[
EF + FE \geq -||EF - E \wedge F|| (E + F),
\]

FIG. 1. Illustration of lattices. Some are decorated: (a), (d), (e), (f), (g) & (i), namely, with additional sites added to original lattices. Original lattices of (a)-(d) are trivalent; original lattices of (e)-(h) are four-valent; the original lattice of (i) is of mixed vertex degrees of 3 and 4.

FIG. 2. Illustration of local structure of decorated lattices: (a) the decorated honeycomb and (b) the decorated square lattice, both with \( n = 2 \).
The ‘right’ set of vertices $E$ lattice and the $E$ ing decorated sites on the edge equivalently the transfer matrix obtained from the ten-

In the above expressions, $E \chi$ decorated AKLT models, it provides an upper bound on $W \hat{\chi}$ the operator $| \uparrow \uparrow \rangle \langle \uparrow \uparrow \uparrow \uparrow |$ representing a maximally entangled state of the form $\phi' s$ inside the dotted square labeled by $n \leq M$. Using the above Lemma and employing tensor-network approaches, the authors of Ref. show elegantly that

$$\chi_n \leq \varepsilon_n \leq \frac{4 \cdot 3^{-n}}{\sqrt{1 - b_{LR}(n)}} + \left( \frac{16 \cdot 3^{-2n}}{1 - b_{LR}(n)} \right) (1 + b_G(n)),$$

where

$$b_G(n) = \frac{4 \cdot 3^{-n}}{q_L(n) q_R(n)} \| E_L \| \| E_R \|,$$

$$b_L(n) = \frac{8 \cdot 3^{-n}}{q_L(n)} \| E_L \|,$$

$$b_R(n) = \frac{4 \cdot 3^{-n}}{q_R(n)} \| E_R \|,$$

$$b_{LR}(n) = b_L(n) + b_R(n) - b_L(n) b_R(n).$$

In the above expressions, $E_L$ is the quantum channel or equivalently the transfer matrix obtained from the tensors $T_L$ associated with the ‘left’ set of vertices $Y_L$ excluding decorated sites on the edge $e = (v, w)$. The $E_R$ (via tensors $T_R$) is associated with the ‘right’ set of vertices $Y_R$. See also Fig. 2a and Fig. 3.

For illustration. More precisely,

$$E_L(B) = \sum_l (T_l^L)^\dagger B T_l^L, \quad E_R(C) = \sum_r T_r^R C(T_r^R)^\dagger.$$

Note that the norms associated with $\| E_L \|$ and $\| E_R \|$ refer to the operator norm by Hilbert-Schmidt norm of matrices, i.e.,

$$\| E \| = \max_B \sqrt{\text{Tr}(E(B)^\dagger E(B))} \sqrt{\text{Tr}(B^\dagger B)},$$

where $B$ is any nonzero square matrix appropriate for the action of $E$ to make sense. Moreover, two matrices are defined $Q_L \equiv E_L(1)$ and $Q_R \equiv E_R(\rho_1)$, and $q_L$ and $q_R$ are their respective minimum eigenvalues. For the proof, we highly recommend Ref. to the readers.

### III. ANALYSIS OF SPECTRAL GAP

The spin-2 entity residing on each square lattice site is composed of four virtual qubits projected onto their symmetric subspace, and the mapping between the physical spin-2 degrees of freedom and the those in the symmetric subspace is as follows,

$$P_{\text{sym}} = |2\rangle\langle\uparrow\uparrow\downarrow\downarrow| + |\downarrow\downarrow\uparrow\uparrow\rangle + |\downarrow\uparrow\uparrow\downarrow\rangle + |\uparrow\downarrow\uparrow\downarrow\rangle$$

where $|m\rangle$’s are eigenstates of $S_z$ operators with eigenvalue $m$. If we consider one square lattice site on the left, then there are corresponding tensors for $P_{m}^L$, which are

$$P_2 = |\uparrow\rangle\langle\uparrow\uparrow|, \quad P_{-2} = |\downarrow\rangle\langle\downarrow\downarrow|,$$

$$P_1 = \frac{1}{2} |\uparrow\rangle\langle\uparrow\downarrow| + \frac{1}{2} |\downarrow\rangle\langle\downarrow\uparrow|,$$

$$P_{-1} = \frac{1}{2} |\uparrow\rangle\langle\downarrow\downarrow| + \frac{1}{2} |\downarrow\rangle\langle\uparrow\uparrow|,$$

$$P_0 = \frac{1}{\sqrt{6}} |\uparrow\rangle\langle\uparrow\downarrow| + \frac{1}{\sqrt{6}} |\downarrow\rangle\langle\downarrow\uparrow|,$$

Because the AKLT state is formed from projecting virtual singlet pairs via the symmetric projectors, we obtain the local tensors describing the spin-2 site on the left as $W_L^L \equiv \sqrt{2}K P_k$, where $K = (|\uparrow\rangle\langle\downarrow| - |\downarrow\rangle\langle\uparrow|)/\sqrt{2}$, and
they are given as follows,

\[
\begin{align*}
W_{L_2}^{L_2} &= -|\downarrow\rangle\langle\uparrow\uparrow\uparrow|, & W_{L_2}^{L_2} &= |\uparrow\rangle\langle\downarrow\downarrow\downarrow|, \\
W_{L_1}^{L} &= \frac{1}{2}(|\uparrow\rangle\langle\uparrow\uparrow\uparrow| - \frac{1}{2}|\downarrow\rangle\langle\uparrow\downarrow\downarrow| + (\langle\uparrow\downarrow\downarrow| + \langle\uparrow\uparrow\uparrow|)), \\
W_{L_1}^{L} &= -\frac{1}{2}(|\downarrow\rangle\langle\downarrow\downarrow\downarrow| + \frac{1}{2}|\uparrow\rangle\langle\uparrow\uparrow\uparrow| + (\langle\uparrow\uparrow\uparrow| + \langle\downarrow\downarrow\downarrow|)), \\
W_{o}^{o} &= -\frac{1}{\sqrt{6}}(|\downarrow\rangle\langle\downarrow\downarrow\downarrow| + \langle\uparrow\uparrow\uparrow| + (\downarrow\uparrow\uparrow|) + (\downarrow\downarrow\uparrow|)).
\end{align*}
\]

See also Fig. 3 for illustration of the local lattice structure and the corresponding tensors. From these, one can easily check that

\[
\sum_{k} W_{L_{k}}^{L_{k}}(W_{L_{k}}^{L_{k}})^{\dagger} = \frac{5}{2} |1\rangle_{C_{2}},
\]

and one can define a quantum channel

\[
E^{\sigma}(B) \equiv \sum_{i} (W_{i}^{L})^{\dagger} BW_{i}^{L}.
\]

One also finds that

\[
E^{\sigma}(\mathbb{I}) = \frac{5}{4} \Pi_{\text{sym}}^{S=3/2},
\]

where \(\Pi_{\text{sym}}^{S=3/2}\) is the projector to the 3-qubit symmetric subspace. At this point it is useful to introduce the two W states used in quantum information so as to simplify the notation,

\[
|w\rangle = \frac{1}{\sqrt{3}}(|\uparrow\uparrow\downarrow| + |\uparrow\downarrow\uparrow| + |\downarrow\uparrow\uparrow|),
\]

\[
|\bar{w}\rangle = \frac{1}{\sqrt{3}}(|\uparrow\downarrow\downarrow| + |\downarrow\uparrow\downarrow| + |\downarrow\downarrow\uparrow|).
\]

The associated dual quantum channel is defined as \(E^{\sigma^{t}}(B) \equiv \sum_{i} W_{i}^{L} B(W_{i}^{L})^{\dagger}\), which maps any three-qubit density matrix to a one-qubit density matrix, and can be written as (assuming \(B\) is hermitian for simplicity)

\[
E^{\sigma^{t}}(B) = c_{0}(B) \mathbb{I} + c_{x}(B) \sigma^{x} + c_{y}(B) \sigma^{y} + c_{z}(B) \sigma^{z},
\]

where the four coefficients \(c\)'s are

\[
c_{0}(B) = \frac{5}{8}(|\uparrow\uparrow\uparrow| |\uparrow\downarrow\downarrow| + |\downarrow\uparrow\uparrow| |\downarrow\downarrow\downarrow|),
\]

\[
+ \frac{5}{8}(|\uparrow\rangle |w\rangle + \langle\bar{w}| B\bar{w})),
\]

\[
c_{x}(B) = -\frac{\sqrt{3}}{8}(|\uparrow\uparrow\uparrow| |\downarrow\downarrow\downarrow| + |\downarrow\uparrow\uparrow| |\downarrow\downarrow\downarrow|),
\]

\[
- \frac{\sqrt{3}}{8}(|\downarrow\rangle |\bar{w}\rangle + \langle\bar{w}| \bar{w})),
\]

\[
\frac{1}{4}(|\uparrow\rangle |\bar{w}\rangle - \langle\bar{w}| B\bar{w})),
\]

\[
ic_{y}(B) = \frac{\sqrt{3}}{8}(|\uparrow\uparrow\uparrow| |\downarrow\downarrow\downarrow| + |\downarrow\uparrow\uparrow| |\downarrow\downarrow\downarrow| + |\downarrow\uparrow\uparrow| |\downarrow\downarrow\downarrow|)
\]

\[
+ \frac{\sqrt{3}}{8}(|\downarrow\rangle |\bar{w}\rangle + \langle\bar{w}| \bar{w})),
\]

\[
\frac{1}{4}(|\uparrow\rangle |\bar{w}\rangle - \langle\bar{w}| B\bar{w})),
\]

\[
\frac{1}{4}(|\downarrow\rangle |\bar{w}\rangle - \langle\bar{w}| B\bar{w})).
\]

Similar to the decorated honeycomb case, \(E^{\sigma^{t}}(B)\) is invariant in permuting \(a, b\) and \(c\) in the special form \(B = a \otimes b \otimes c\), and this simplifies the calculation. Let us use lower-case \(s\) to denote the spin-1/2 operators \(s^{u} = \sigma^{u}/2\) and \(\rho_{1} = \mathbb{I}/2\). One can then by direct calculation show that

\[
E^{\sigma^{t}}(\rho_{1} \otimes \rho_{1} \otimes \rho_{1}) = \frac{5}{8} \rho_{1},
\]

\[
E^{\sigma^{t}}(s^{u} \otimes s^{u} \otimes s^{u}) = \frac{1}{8} s^{u},
\]

\[
E^{\sigma^{t}}(s^{u} \otimes s^{v} \otimes s^{w}) = \frac{1}{24} s^{u}, \text{ for } u \neq v,
\]

\[
E^{\sigma^{t}}(s^{u} \otimes s^{v} \otimes s^{w}) = 0, \text{ for } u \neq v \neq w,
\]

\[
E^{\sigma^{t}}(\rho_{1} \otimes s^{u} \otimes s^{v}) = \frac{5}{24} \delta_{uv} \rho_{1},
\]

\[
E^{\sigma^{t}}(\rho_{1} \otimes \rho_{1} \otimes s^{u}) = \frac{5}{24} s^{u}.
\]

It is convenient to introduce

\[
\Lambda^{u} \equiv \mathbb{I} \otimes s^{u} \otimes s^{v} + s^{u} \otimes \mathbb{I} \otimes s^{v} + s^{u} \otimes s^{v} \otimes \mathbb{I},
\]

and by direct calculation one can re-write Eq. (20) as

\[
E^{\sigma}(\mathbb{I}) = \frac{5}{4} \Pi_{\text{sym}}^{S=3/2} = \frac{5}{8} (\mathbb{I} \otimes \mathbb{I} \otimes \mathbb{I} + \frac{4}{3} \sum_{u=x,y,z} \Lambda^{u}),
\]

and this will allow us later to deduce \(E^{\sigma}\) from the actions of \((E^{\sigma})^{t}\) in Eqs. (28) by fixing the overall scale.

It is convenient to express the channel and its dual in the form of a matrix or sometimes called the superoperator form. Thus, any matrices, such as \(\sigma\), that the channels act on will be written in terms of vectors, such
as $|\sigma\rangle$. Moreover, the inner product between two such `vectors' becomes $\langle |\sigma\rangle |\rho\rangle \equiv \text{Tr}(\sigma^\dagger \rho)$. Note that in this definition $\langle |\rho_1\rangle |\rho\rangle = 1$. Then exploiting the permutation invariance, one can use the trick used in Ref. [1], by using the action of the dual channel $(E^\circ)^* \equiv E^\circ_{\text{dual}}$ in Eq. [25] and fixing the overall scale via Eq. [30], to deduce the action of $E^\circ$ and write it in the `superoperator' form as

$$E^\circ = 5|\rho_1\rangle \langle \rho_1| \sum_{u=x,y,z} |s^u s^u\rangle \langle s^u| + \sum_{u=x,y,z} \left( \sum_{v \neq u} (|s^u s^u v\rangle + |s^v s^u v\rangle + |s^v s^u v\rangle) \langle s^u| \right)$$

(31)

where we have suppressed the $\otimes$ symbols. It is also possible to calculate $E^\circ$ directly from its definition in Eq. [19], but the trick above helps to express $E^\circ$ in terms of the sum of the product forms.

From the results of Ref. [1], the channel $E^\circ$ along a decorated spin-1 sites,

$$E^\circ(B) \equiv \sum_{\nu} V^\dagger_{\nu} \cdots V^\dagger_{1} BV_{1} \cdots V_{\nu}$$

(32)

can be calculated to be

$$E^\circ = |1\rangle \langle 1| + \sum_{u} |s^u\rangle \langle s^u|$$

(33)

and thus the combined channel from the left is

$$E_L = (E^\circ \otimes E^\circ \otimes E^\circ) E^\circ_{\text{dual}}$$

(34)

$$= 5 \left( \prod_{u=x,y,z} |s^u s^u\rangle \langle s^u| \right)$$

$$+ \left( \prod_{u=x,y,z} (|s^v s^u v\rangle + |s^v s^u v\rangle + |s^v s^u v\rangle) \right)$$

$$- \left( \prod_{u=x,y,z} (|s^v s^u v\rangle + |s^v s^u v\rangle + |s^v s^u v\rangle) \right)$$

$$- \left( \prod_{u=x,y,z} (|s^v s^u v\rangle + |s^v s^u v\rangle + |s^v s^u v\rangle) \right)$$

$$+ \left( \prod_{u=x,y,z} (|s^v s^u v\rangle + |s^v s^u v\rangle + |s^v s^u v\rangle) \right)$$

$$- \left( \prod_{u=x,y,z} (|s^v s^u v\rangle + |s^v s^u v\rangle + |s^v s^u v\rangle) \right)$$

(35)

where $\Lambda^u$ was introduced in Eq. [29] and here we introduce its vectorized form $|\Lambda^u\rangle \equiv |s^u s^u\rangle + |s^v s^u v\rangle + |s^v s^u v\rangle$ and $|\Omega^u\rangle \equiv |s^u s^u\rangle + |s^v s^u v\rangle + |s^v s^u v\rangle$, as well as $|\Theta^u\rangle \equiv \sum_{v \neq u} (|s^u s^v v\rangle + |s^v s^u v\rangle + |s^v s^u v\rangle)$. We note that the transfer operator or the quantum channel $E_L$ is completely positive, which can be checked by directly diagonalizing the corresponding Choi matrix [22] and seeing that they are positive.

Next, we evaluate the operator norm for $E_L$. To do that we note that $||\prod_{u} |s^u\rangle \langle s^u| ||^2 = 1/8$, $||s^u s^v\rangle ||^2 = 1/8$, $||\Lambda^u\rangle ||^2 = 3/2$, $||\Omega^u\rangle ||^2 = 6$, and $||\Theta^u\rangle ||^2 = 3/4$. Since $E_L$ is ‘diagonal’ in $|\rho_1\rangle$ and $|s^u\rangle$ basis regarding its domain, we can take without loss of generality $\phi = a_0 |\rho_1\rangle + a_1 \cdot s$ or its vectorized version $|\phi\rangle = a_0 |\rho_1\rangle + \sum_{u=x,y,z} a_u |s^u\rangle$, and then maximize the following expression to obtain the norm

$$||E_L||_{\text{op}} = \max_{a_0} ||E_L(\phi)|| / ||\phi||,$$

(36)

for which we obtain

$$||E_L||_{\text{op}} = \frac{5}{4} \sqrt{1 + 3^{-4n}}.$$

(37)

We also evaluate the operator $Q_L \equiv E_L(1)$, and obtain it in the matrix form (instead of $|\cdots\rangle\rangle$)

$$Q_L = \frac{5}{8} \prod_{u=x,y,z} + \frac{5}{6} \cdot \frac{3}{2n} \sum_{u} \Lambda^u,$$

(38)

One can diagonalize $Q_L$ and obtain its spectrum (noting $\sum_{u} \Lambda^u$ has eigenvalues $\pm 3/4$)

$$\text{spec}(Q_L) = \left( \frac{5}{8} \pm \frac{5}{6} \cdot \frac{3}{2n} \right).$$

(39)

Therefore, the smallest eigenvalue $q_L$ of $Q_L$ is

$$q_L = \frac{5}{8} - \frac{5}{6} \cdot \frac{3}{2n}.$$

(40)

Hence we can calculate the associated $b_L(n) = 8a(n)||E_L|| / q_L$ and obtain

$$b_L(n) = \frac{16 \cdot 3^{-n} \sqrt{1 + 3^{-4n}}}{1 - 3^{-2n}},$$

(41)

where $a(n) = ||E^n - 1|| / ||\rho_1||$ was previously obtained in Ref. [1] to be $3^{-n}$; but one can also calculate $a(n)$ directly from Eq. [33].

Next, we examine the channel coming from the right square-lattice site. The onsite tensors are defined as $W^R_k \equiv 2\sqrt{2}(K \otimes K \otimes K)P^R_k$, and one finds that

$$W^R_2 = -(W^L_2)^\dagger,$$

(42)

$$W^R_1 = (W^L_1)^\dagger,$$

(43)

$$W^R_0 = -(W^L_1)^\dagger.$$
between the minimum eigenvalues of $Q_R$ and $Q_L$ is $q_R = q_L/2$. We therefore obtain
\begin{align}
b_R(n) &= 4a(n)\| E_R \|/q_R = b_L(n), \\
b_G(n) &= 4a(n)\| E_L \|/q_R = 8a(n)/q_L^2.
\end{align}

The injectivity of the mappings $\Gamma_{G_{L/R-c_n}}$ and $\Gamma_G$ for the corresponding matrices $B$, $C$, $D$ to the respective quantum states,
\begin{align}
\Gamma_{G_{L-c_n}}(B) &\equiv \sum_{i_1, \ldots, i_n} \text{Tr}[BV_{i_n} \cdots V_{i_1} T^L_i |l\rangle \otimes |i_1, \ldots, i_n\rangle], \\
\Gamma_{G_{R-c_n}}(C) &\equiv \sum_{i_1, \ldots, i_n, r} \text{Tr}[CT^R_r V_{i_n} \cdots V_{i_1} |i_1, \ldots, i_n\rangle \otimes |r\rangle_R], \\
\Gamma_G(D) &\equiv \sum_{i, i', r, s} \text{Tr}[DT^R_r V_{i_n} \cdots V_{i_1} T^L_i |l\rangle \otimes |i_1, \ldots, i_n\rangle \otimes |r\rangle_R],
\end{align}

depends on whether $1 - b_{L/R}(n) > 0$ and $1 - b_G(n) > 0$, respectively; see Ref. [1]. In the above equations, $T^L_i$ and $T^R_i$ denote tensors from the left and right sides, respectively, $|l\rangle_L$ and $|r\rangle_R$ are basis states for the left and right sides, respective, and $V_i$ denotes the tensor for one spin-$1$ site that decorates the edge ($n$ is the total number of such sites); see Fig. 6. We have checked that $\Gamma_{G_{L-c_n}}$ and $\Gamma_{G_{R-c_n}}$ are both injective for $n \geq 3,

\begin{table}[h]
\centering
\begin{tabular}{ |c|c|c|c|}
\hline
$n$ & degree 3 & degree 4 & mixed degrees 3 & 4 \\
\hline
1 & 0.4775328889 & 0.5234369088 & 0.5001917602 \\
2 & 0.118337500 & 0.1218467396 & 0.120794787 \\
3 & 0.038437328 & 0.038903328 & 0.0385700977 \\
4 & 0.012446109 & 0.0124961718 & 0.0124710706 \\
\hline
\end{tabular}
\caption{$\varepsilon_n$ for both the decorated honeycomb, square lattices and the lattice with mixed degrees 3 & 4 (with 10 digits of accuracy presented). If $\varepsilon_n < 1/3$ for the decorated honeycomb case, then we are sure that the corresponding AKLT model is gapped. For the decorated square lattice and the mixed-degree one, if $\varepsilon_n < 1/4$, then we are sure that the corresponding AKLT model is gapped. From this table, we conclude that the AKLT models are gapped on both types of decorated lattices for $n \geq 2$.}
\end{table}

but $\Gamma_G$ is injective for $n \geq 4$. In Ref. [1], $b_{L/R}(n) \equiv b_L(n) + b_R(n) - b_L(n)b_R(n) = 2b_L(n) - b_L(n)^2$, and it was shown that the important quantity $\varepsilon_n$ that suffices to deduce a finite spectral gap when $\varepsilon_n < 1/4$ (as the coordination number for the square lattice is 4 compared to 3 in the hexagonal lattice), is upper bounded by

$$
\varepsilon_n \leq \frac{4a(n)}{\sqrt{1 - b_{L/R}(n)}} + \left(\frac{4a(n)}{\sqrt{1 - b_{L/R}(n)}}\right)^2 (1 + b_G(n)).
$$

Thus, we have

$$
d(n) = \frac{4a(n)}{|1 - b_{L/R}(n)|} + \left(\frac{4a(n)}{1 - b_{L/R}(n)}\right)^2 (1 + b_G(n)).
$$

We can thus prove that the AKLT models on the decorated square lattice are gapped with $n \geq 4$, as shown in Fig. 6.

We also performed numerical calculations for $\varepsilon_n$ for both the decorated honeycomb and square lattice, as well as one with mixed degrees, and confirmed that for both $n = 2$ and $n = 3$ the AKLT models are also gapped. The numerical results are shown in Table IV We describe our methods in Sec. IV.
IV. COMMENTS ON THE HONEYCOMB CASE AND BEYOND

A. Norm of $E_L$ in the honeycomb case

For the honeycomb case, the channel from the left was calculated in Ref. [1]

$$E_L = |\mathbb{1}\mathbb{1}\rangle\langle\rho_1| + 2\frac{(-1)^n + 1}{3^n} \sum_u |\Omega^u\rangle\langle s^u|$$

$$+ \frac{4}{3^{2n + 1}}|\vec{s} \cdot \vec{s}|\langle\rho_1|,$$

(49)

where $|\Omega^u\rangle = |s^u\mathbb{1}\rangle + |\mathbb{1}s^u\rangle$. To calculate the norm, we note that $||\mathbb{1}\mathbb{1}||^2 = 4$, $||s^u s^u||^2 = 1/4$ (hence $||\vec{s} \cdot \vec{s}||^2 = 3/4$), $||\Omega^u||^2 = 2$. Since $E_L$ is ‘diagonal’ in $|\rho_1\rangle$ and $|s^u\rangle$, we take without loss of generality $\phi = a_0 \rho_1 + \vec{a} \cdot \vec{s}$ or its vectorized version $|\phi\rangle = a_0 |\rho_1\rangle + \sum_{u=x,y,z} a_u |s^u\rangle$, and then maximize the following expression to obtain the norm

$$||E_L||_{op} = \max_{\phi} ||E_L(\phi)||/||\phi||.$$  

(50)

By direct calculation we have

$$||E_L(\phi)||^2 = |a_0|^2(1 + 3^{-4n-1}) + \sum_u 2|a_u|^2 \cdot 3^{-2n},$$

(51)

and $||\phi||^2 = (|a_0|^2 + \sum_u|a_u|^2)/2$, the norm is thus $||E_L|| = \sqrt{2(1 + 3^{-4n-1})}$. Thus, we have (noting $q_R = 2q_R = 1 - 3^{-2n}$ from Ref. [1])

$$b_L(n) = b_R(n) = 8 \cdot 3^{-n} \sqrt{2(1 + 3^{-4n-1})},$$

$$b_G(n) = 16 \cdot 3^{-n} \frac{1 + 3^{-4n-1}}{(1 - 3^{-2n})^2} = \frac{3^n}{8} b_L(n)^2.$$  

(52)

(53)

Therefore, the upper bound $d_{HC}(n)$ on $\varepsilon_n$ (and hence $\chi_n$) is given by

$$d_{HC}(n) = 4 \cdot 3^{-n} \left|\frac{1}{1 - b_L(n)} + \left(\frac{4 \cdot 3^{-n}}{1 - b_L(n)}\right)^2 \left(1 + b_G(n)\right)\right|.$$  

(54)

So we see that the injectivity of $\Gamma_{L-C_n}$ holds for $n \geq 3$, but the gap is only proven analytically for $n \geq 4$; see e.g. Fig. 7.

B. Other trivalent lattices

Since the proof in the decorated honeycomb case only relies on the local structure of the two vertices on the original lattice and the corresponding tensors (see Fig. 3 for illustration), a moment of thought will convince one that it also holds exactly for other trivalent lattices with decoration; see Fig. 4 for illustration of other lattices. Therefore for all trivalent lattices (which can be of any dimensions, such as 3D) the AKLT models on the corresponding decorated lattices will also be gapped if $n \geq 4$, where again $n$ is the number of spin-1 sites added to decorate an edge. In fact, for each original edge, the number of decorated sites $n_e$ can be different, and the corresponding AKLT model will still be gapped as long as $n_e \geq 4$. Numerically these are improved to $n_e \geq 2$.

C. Other lattices of vertex degree 4

By the same token, since we have proven that the AKLT models on the decorated square lattices are gapped if $n \geq 4$, this will also hold for any other decorated lattices, whose original vertex degree is 4; see Fig. 1g&h for illustration of such other lattices. Numerically these are improved to $n \geq 2$. AKLT states on the 3D diamond lattice (also four-valent) and the associated decorations are also universal [16] [17], and the significance is that these 3D resource states are likely to provide fault-tolerance similar to the 3D cluster state [18]. Therefore, the decorated diamond lattices host AKLT models that are gapped for $n \geq 2$, and the corresponding ground states are also universal and provides topological protection for MBQC.

D. Other lattices of fixed vertex degree

We conjecture that for any lattices of fixed vertex degree, the AKLT models on the corresponding decorated lattices will be gapped, as long as $n$ is large enough. The intuition comes from that for large $n$, it is essentially many long spin-1 AKLT chains incident on some vertices, which act as local perturbation. For $n$ sufficiently large, the perturbation is of measure zero as $n \rightarrow \infty$. The analytic approach of Ref. [1] and our numerical method below can be applied to these.
Thus, we obtain the corresponding function $d(n) - 1/4$ instead of $d^{\text{mix}}(n) - 1/3$ to check the gappedness.

E. Lattices of mixed vertex degrees

A natural question to ask is for AKLT models residing on decorated lattices, whose original lattice is of mixed vertex degrees. It is likely that they will be gapped as long as $n$ is sufficiently large.

Let us consider the lattice (i) in Fig. 1 whose original lattice has mixed vertex degrees of 3 and 4. Take the left original site to be of degree 3 and the right original site of degree 4. We have to evaluate $b_L(n)$, $b_R(n)$, $b_{LR}(n)$, $E_L$ and $E_R$, and they can be obtained partly from the honeycomb case and partly from the square lattice case,

$$b_L(n) = b_{L}^{HC}(n) = 8 \cdot 3^{-n} \sqrt{2(1 + 3^{-4n-1})} / (1 - 3^{-2n}),$$

$$b_R(n) = b_{R}^{SQ}(n) = 16 \cdot 3^{-n} \sqrt{1 + 3^{-4n}} / (1 - 3^{-2n}),$$

$$b_{LR}(n) = b_L(n) + b_R(n) - b_L(n)b_R(n),$$

$$||E_L|| = ||E_{L}^{HC}|| = \sqrt{2(1 + 3^{-4n-1})},$$

$$||E_R|| = ||E_{R}^{SQ}|| = 5 / 4 \sqrt{1 + 3^{-4n}},$$

$$b_G(n) = 8 \cdot 3^{-n} ||E_L|| ||E_R|| / (q_{L}^{HC} q_{R}^{SQ}),$$

$$q_{L}^{HC} = 1 - 3^{-2n}, \quad q_{R}^{SQ} = 5 / 16 - 5 / 16 \cdot 3^{2n}.$$  (61)

Thus, we obtain the corresponding function $d(n)$ for the mixed-degree lattice,

$$d^{\text{mix}}(n) = \frac{4 \cdot 3^{-n}}{\sqrt{1 - b_{LR}(n)}} + \left( \frac{4 \cdot 3^{-n}}{\sqrt{1 - b_{LR}(n)}} \right)^2 (1 + b_G(n)).$$  (62)

We see that the AKLT models are gapped for $n \geq 4$ for the decorated lattices, as checked in Fig. 8. Numerically these are improved to $n_e \geq 2$; see Table II.

V. NUMERICAL METHODS

Here we explain our numerical approach for producing the numerics for $\varepsilon_n$ in Table II, which was derived based on Lemma 6.3 of [7]. The analytical results in the previous sections provide only upper bounds on $\varepsilon_n$, as inequalities such as operators norms and Schwarz in equalities were used in deriving, e.g., Eq. (11). As we have seen, the analytics can only establish non-zero gap for $n \geq 4$, but our numerical evaluation of $\varepsilon_n$ was able to push the gappedness to $n \geq 2$.

We begin by noting part (1) of the Lemma, which determines that

$$\varepsilon \equiv \| EF - E \wedge F \| = \|(1 - E)(1 - F) - (1 - E) \wedge (1 - F) \|,$$  (63)

where $E \wedge F$ projects onto the intersection of images $EH \cap FH$ and, likewise, $E \vee F$ projects onto the sum of $EH + FH$, or $(EH^\perp + FH^\perp)^\perp$. From here on we will use $E \equiv 1 - P_v$ and $F \equiv 1 - P_w$ rather than their complements, which as we will see will be useful because $P_v$ and $P_w$ are high-dimensional projectors and their complements are low-dimensional.

Here we also review the findings that lead the source to part (2) of the Lemma. In doing so, we will diverge from the source by not quotienting out $EH \cap FH$ and $EH^\perp \cap FH^\perp$ (i.e. setting $E \wedge F = 0$ and $E \vee F = \infty$), as we ultimately will be working partly within those spaces. We consider the eigenvalue equation

$$(E + F)\Upsilon = (1 - \alpha)\Upsilon.$$  (64)

Clearly, as $E$ and $F$ are Hermitian operators whose eigenvalues belong to $\{0, 1\}$, the range of possible values of $\alpha$ is $[-1, 1]$. Moreover, we note that $\alpha = -1$ corresponds exactly to the subspace $EH \cap FH$, whereas $\alpha = 1$ corresponds exactly to the subspace $EH^\perp \cap FH^\perp$. Therefore, for $\alpha \neq \pm 1$, we can uniquely write $\Upsilon = \varphi + \psi$ for

$$\varphi \in V_E \equiv EH \cap (EH \cap FH)^\perp,$$

$$\psi \in V_F \equiv FH \cap (EH \cap FH)^\perp,$$  (65)

(i.e. as within the direct sum of two subspaces $V_E \subset EH$ and $V_F \subset FH$ which, while nonintersecting, will not generically be orthogonal.) We therefore can determine

$$(E + F)(\varphi + \psi) = (1 - \alpha)(\varphi + \psi)$$

$$E\varphi + E\psi + F\varphi + F\psi = (1 - \alpha)\varphi + (1 - \alpha)\psi$$

$$(\varphi + E\psi) + (\psi + F\varphi) = (\varphi - \alpha\varphi) + (\psi - \alpha\psi).$$  (66)

From the aforementioned uniqueness of the decomposition, this implies $E\psi = -\alpha\varphi$ and $F\varphi = -\alpha\psi$. From this we can directly compute

$$(E + FE)(\varphi + \psi) = -\alpha(1 - \alpha)(\varphi + \psi)$$  (67)

Moreover we note that direct calculation gives us $EF + FE|_{EH\cap FH} = 0$ and $EF + FE|_{EH^\perp\cap FH^\perp} = 2$. That is, consideration of individual eigenspaces gives us

$$EF + FE \geq -\max(\{\alpha\} \setminus \{1\})(E + F).$$  (68)
We will then follow the original proof of part (1) of the Lemma in demonstrating

**Proposition 1** The inequality

\[ EF + FE \geq -\varepsilon(E + F) \]  

(69)

is optimized by \( \varepsilon = \max(\{\alpha \} \setminus \{1\}) = \|EF - E \wedge F\| \). In particular, \(-\varepsilon \) is the least nontrivial eigenvalue of \( E + F \).

The operator norm \( \|O\| \) is equivalent to the supremal real value of \( \langle \Phi|O|\Psi\rangle \) for unit \( \Phi, \Psi ; \) in particular such that \( O\Psi = \|O\|\Phi \) and \( \|O\|\Psi = O^1\Phi \). In finding \( \Psi \), we note that \( EF - E \wedge F \) vanishes on both \( FH^\perp \) and \( EH \cap FH^\perp \); i.e. \( \Psi \) is orthogonal to these spaces and in particular \( \Psi \in V_F \). Likewise, the Hermitian transpose vanishes on \( EH \cap FH^\perp \) so that we should find \( (EF - E \wedge F)\Psi \in V_F \); in particular, \( \Phi \in V_E \). Thus we can write \( EF\Psi = E\Psi = \varepsilon\Phi \) and \( (EF)^\dagger \Phi = F\Phi = \varepsilon\Phi \). It follows that

\[ (EF + FE)(\Psi - \Phi) = (\varepsilon - \varepsilon^2)(\Psi - \Phi) = -\varepsilon(E + F)(\Psi - \Phi) \]  

(70)

Moreover for any eigenvector \( \Psi \) of \( E + F \) with eigenvalue \( 1 - \alpha \in (0, 2) \), decomposed as above into \( \varphi + \psi \), \( (EF - E \wedge F)\psi = EF\psi = -\alpha\varphi \). This implies that \( \|EF - E \wedge F\| \geq |\alpha| \) for \( \alpha \neq \pm 1 \); that is \( \varepsilon = \max(\{\alpha \} \setminus \{1\}) \).

Therefore, determining \( \varepsilon \) is equivalent to determining the least nontrivial eigenvalue of \( E + F \). We now demonstrate that we can simplify \( E + F \) and, by extension, reduce the complexity of this calculation.

Consider a projector \( A \), with the properties \( EA = AE = E \) (i.e. \( AH \supset E\mathcal{H} \)) and \([A, F] = 0 \). (In particular, we will be interested in a projector defined on the sites \( Y_v \setminus Y_w \).

**Proposition 2** For an eigenvector \( \Psi \) of \( E + F \) with eigenvalue \( 1 - \alpha, A \notin \{-1, 0, 1\}, AT = \Psi \).

As above, we write \( \Psi = \varphi + \psi \) with \( \varphi \in V_E \) and \( \psi \in V_F \), so that \( E\Psi = -\alpha\varphi \) and \( F\Psi = -\alpha\varphi \); in particular \( FE\Psi = \alpha^2\psi \). Manifestly \( A\varphi = \varphi \) as \( \varphi \in E\mathcal{H} \); meanwhile, since \( \alpha \neq 0 \) we can write

\[ A\psi = \alpha^{-2}AFE\psi = \alpha^{-2}FAE\psi = \alpha^{-2}FE\psi = \psi. \]

We use \( A \) to project onto a lower-dimensional subspace \( \mathcal{H}' \); that is we take \( U_A : \mathcal{H} \rightarrow \mathcal{H}' , \) for \( \mathcal{U}_A U_A = A \) and \( U_A U_A = 1 \). Setting \( E' = U_A E U_A \) and \( F' = U_A F U_A \). That \( E' \) and \( F' \) are projectors follows directly from the fact that \( E \) and \( F \) commute with \( A \). Moreover,

**Proposition 3** \( \|E'F' + E' \wedge F'\| = \|EF + E \wedge F\| \)

We do this by examining the spectrum of \( E' + F' \), as in Prop. 1. Since \( A \) commutes with \( E \) and \( F \), we find that

\[ (E + F)U_A^\dagger \Psi' = (E + F)U_A^\dagger(U_A U_A) \Psi' \]

\[ = A(E + F)U_A^\dagger \Psi' = U_A^\dagger(E' + F') \Psi'; \]

that is, for any eigenvector \( \Psi' \) of \( E' + F' \), \( U_A^\dagger \Psi' \) is an eigenvector of \( E + F \) with the same eigenvalue. Put otherwise, the spectrum of \( E' + F' \) is a subset of that of \( E + F \). Then, by Prop. 2 only the degeneracies of eigenvectors 0, 1, and 2 are affected; in particular the least nontrivial eigenvector is preserved.

We additionally note that, for a fourth projector \( B \) commuting with \( E \) and \( A \) and satisfying \( FB = BF = F \), \( B' = U_A BU_A \) satisfies the same hypotheses for \( E' \) and \( E' \). Decomposing \( B' = U_B U_B, U_B U_B = 1 \), we can therefore move to a still smaller space \( \mathcal{H}'' \equiv B\mathcal{H}' \) and perform our analysis on \( E'' = U_B E' U_B \) and \( F'' = U_B F' U_B \). The method we use to efficiently exploit these conclusions is as follows:

1. Determine \( E = 1 - P_v \) as follows:

   (a) Construct the tensor corresponding to the portion of the AKLT state defined on \( Y_v \), containing both physical and virtual indices (in the honeycomb-lattice case, \( 3n + 1 \) physical and 3 virtual; in the square-lattice case, \( 4n + 1 \) physical and 4 virtual indices).

   (b) Collect the physical and virtual indices, in order to turn the representation into a matrix

   \[ \Psi \in \mathcal{H}_{\text{phys}} \otimes \mathcal{H}_{\text{virt}}. \]

   (c) Using the singular-value decomposition \( \Psi = W_s V_{11} \), then \( E = WW^\dagger \).

2. Taking \( U_E = W_s^\dagger \), we can repeat this process to define isometries \( U_F \) on \( Y_w \), \( U_A \) on \( Y_v \setminus Y_w \), and \( U_B \) on \( Y_w \setminus Y_v \).

3. Write \( U_E' = U_A U_B \) and \( U_F' = U_B U_A \) (as it may be prohibitively memory-expensive to represent even \( E \) and \( F \) in full).

4. Then \( E'' = U_B^\dagger U_B \) and \( F'' = U_B^\dagger U_B \) can be used to extract \( \varepsilon \) by diagonalizing \( E'' + F'' \).

**VI. CONCLUDING REMARKS**

We have followed the elegant approach by Abdul-Rahman et al. [1] and proved analytically that the decorated square lattices with \( n \geq 4 \) host AKLT models with finite spectral gap, similar to the results of the decorated honeycomb case. Our numerical approach allows to show that the AKLT models on both decorated lattices are gapped even for \( n = 2 \) and \( n = 3 \). The results of the nonzero spectral gap also hold for any other decorated lattices, whose original ones are of fixed vertex degree 3 or 4. But we have also commented and speculated on other lattices. In particular, using the results from both the decorated honeycomb and square lattice, we also show analytically that AKLT models on decorated lattices, whose original one is of mixed vertex degrees 3 and 4, are also gapped for \( n \geq 4 \). This is improved
numerically to $n \geq 2$. Regarding the spectral gap for the AKLT models on the original honeycomb or square lattice, we also share the same view as the authors of Ref. [1], i.e. to establish their spectral gap will require a different and maybe novel approach. However, some insight may be obtained if one can make progress analytically on the cases of $n = 1, 2, 3$ and in particular check whether $n = 1$ case is gapped or not, for which we strongly suspect that it is gapped.

The AKLT models have spin rotational symmetry but deformation that breaks the full SO(3) symmetry were considered, such as the deformed AKLT models in Refs. [23, 24]. Can we employ similar approach to prove the spectral gap for the deformed models on the decorated lattices? Or perhaps other ideas from tensor network can be useful, such as in Ref. [25]. Some of deformed AKLT states were also previously shown to provide universal resource for MBQC within some finite range of deformation [26, 27]. These deformed models also have interesting phase diagram [23, 24]. It is worth mentioning that some related 2D Hamiltonians mixing the AKLT models and the cluster-state models were also shown to have finite spectral gap [30], but the spectral gap in the exact AKLT limit still cannot be proved.

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