



Improved Approximation Algorithms for the EPR Hamiltonian

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Abstract

The EPR Hamiltonian is a family of 2-local quantum Hamiltonians introduced by King [18]. We introduce a polynomial time $\frac{1+\sqrt{5}}{4} \approx 0.809$ -approximation algorithm for the problem of computing the ground energy of the EPR Hamiltonian, improving upon the previous state of the art of 0.72 [17].

2012 ACM Subject Classification Theory of computation → Approximation algorithms analysis

Keywords and phrases Approximation Algorithms, Quantum Local Hamiltonian

Digital Object Identifier 10.4230/LIPIcs.APPROX/RANDOM.2025.24

Category APPROX

Supplementary Material *Software (Source code)*: <https://github.com/anshnagda/EPR-algorithm>
archived at `swh:1:dir:0c84d61b32f7cc919be9311c24e8136b0e3412f1`

1 Introduction

Constraint Satisfaction Problems (CSPs) are a central class of computational problems in NP, capturing a wide range of decision problems where the goal is to determine whether there exists an assignment to variables that satisfies a given set of constraints. In the quantum setting, the analogous problem is known as the *local Hamiltonian problem* which is the central computational problem for the complexity class QMA. In this problem, one is given a local Hamiltonian of the form

$$H = \sum_{i \in [m]} h_i,$$

where each term $h_i \in \mathbb{C}^{2^n \times 2^n}$ is a Hermitian matrix over n qubits that only acts nontrivially on $O(1)$ qubits. Given a (mixed) quantum state ρ , we say that the energy of ρ is $\text{tr}(\rho \cdot H)$. In the maximization version of the problem, the objective is to compute the maximum possible energy achieved by any state, which we call the *ground state energy*¹. Note that the ground state energy coincides with the maximum eigenvalue of H :

$$\lambda_{\max}(H) = \max_{\rho \geq 0, \text{tr}(\rho)=1} \text{tr}(\rho \cdot H).$$

We remark that max-CSPs can be thought of as a special case of the local Hamiltonian problem where h_i is a diagonal $2^n \times 2^n$ matrix whose (x, x) entry indicates whether or not a particular predicate is satisfied by x viewed as an assignment of n Boolean variables. In this case, it is immediate that the ground state energy is equal to the maximum number of clauses that can be satisfied by any assignment, and is achieved by the product state $|x^*\rangle\langle x^*|$ where x^* is the optimal assignment.

¹ This is a slight deviation from the usual notion of the ground state being the *minimum* energy state. We remark that both the notions are equivalent up to replacing H by $-H$; we use the maximization notion because it is notationally convenient.



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Approximation, Randomization, and Combinatorial Optimization. Algorithms and Techniques (APPROX/RANDOM 2025).

Editors: Alina Ene and Eshan Chattopadhyay; Article No. 24; pp. 24:1–24:9



Leibniz International Proceedings in Informatics

Schloss Dagstuhl – Leibniz-Zentrum für Informatik, Dagstuhl Publishing, Germany

Computing the ground state energy of a generic local Hamiltonians is computationally infeasible (QMA-hard), so we focus on *approximating* it in this work. Let \mathcal{F} be a family of local Hamiltonians. For $\alpha \in [0, 1]$, an α -*approximation algorithm* for \mathcal{F} is a classical algorithm² that, upon input $H \in \mathcal{F}$, outputs a description of a (mixed) state ρ achieving energy

$$\text{tr}(\rho \cdot H) \geq \alpha \cdot \lambda_{\max}(H).$$

In this work, we consider the EPR Hamiltonian family $\mathcal{F} = \text{EPR}$ which was formally introduced by King [18]. A Hamiltonian $H \in \text{EPR}$ is parametrized by a weighted graph given as a symmetric matrix $w \in \mathbb{R}_{\geq 0}^{n \times n}$, and is defined as

$$H = \sum_{i < j \in [n]} w_{ij} E_{ij},$$

where E_{ij} is a projection onto the EPR state $|\text{EPR}\rangle = \frac{|00\rangle + |11\rangle}{\sqrt{2}}$ on qubits i and j tensored with identity on the rest.

These Hamiltonians naturally arise in the study of quantum systems such as the antiferromagnetic Heisenberg model on lattices and the XXZ model, which have been extensively studied in the physics literature (e.g. [25, 7, 21, 5]).

From the point of view of computational complexity, the EPR Hamiltonian provides perhaps the simplest example of a local Hamiltonian that exhibits new challenges beyond traditional CSP theory. To illustrate this, one can show that among all product states, the one achieving maximal energy is always the trivial state $\rho = |0^n\rangle\langle 0^n|$. This is in contrast to the “diagonal” case of CSPs in which the optimal state is equivalent to the optimal product state. As a result, the main challenge with the EPR Hamiltonian reduces to understanding the entanglement structure of the ground state.

Prior to our work, King [18] obtained a $1/\sqrt{2}$ -approximation for the EPR Hamiltonian, which was later slightly improved to 0.72 [17]. Our main result is an improved approximation algorithm for EPR.

► **Theorem 1.** *There is a polynomial time $\frac{1+\sqrt{5}}{4} \approx 0.809$ -approximation algorithm for the EPR problem.*

► **Remark 2.** In concurrent work, Apte et al. [3] achieved the same approximation ratio of $\frac{1+\sqrt{5}}{4}$ for the EPR Hamiltonian using a different algorithm and analysis.

1.1 Related work

The study of approximation algorithms for local Hamiltonian problems was initiated by Bravyi, Bansal, and Terhal [4] and Gharibian and Kempe [11] which have since been followed by a sequence of works (e.g. [9, 8, 14, 6]).

A line of work initiated by Gharibian and Parekh [12] studies approximation algorithms for a closely related problem to the EPR Hamiltonian, called Quantum Max Cut [23, 1, 24, 19, 18, 15, 28, 26]. The best known results in the literature are an algorithm showing an approximation ratio of 0.611 [3] and a (conditional) hardness result ruling out approximation ratios beyond 0.956 [16]. This leaves a large range of possible values for the optimal approximability by polynomial time algorithms.

² For the purposes of this paper we only consider classical algorithms, but one can also consider quantum algorithms.

For bipartite instances of the EPR Hamiltonian where one part has $O(1)$ vertices, Takahashi et al. [27] devised a polynomial time approximation scheme (PTAS). For general bipartite instances of the EPR Hamiltonian, [13] devised a 0.816-approximation algorithm.

2 Algorithm

2.1 An upper bound on $\lambda_{\max}(H)$

We will begin by describing an efficiently computable upper bound on $\lambda_{\max}(H)$. Let us denote by $\text{LP}(w)$ the optimal value of the following linear program, known as the *fractional matching LP*:

$$\begin{aligned} & \max \sum_{i < j} w_{ij} \cdot x_{ij} \\ \text{s.t. } & \sum_{j \neq i} x_{ij} \leq 1 \quad \text{for all } i \in [n] \\ & x_{ij} \geq 0 \quad \text{for all } i, j \in [n] \end{aligned}$$

Let $x = (x_{ij})_{i < j}$ be an optimal solution to the above LP. We say that the *LP energy* on edge $\{i, j\}$ is $\tilde{E}_{ij} = \frac{1+x_{ij}}{2}$.

The *star bound*, proved by Anshu-Gosset-Morenz [1], gives a way to bound the ground state energy $\lambda_{\max}(H)$ in terms of the above linear program. We will need a version of this bound that applies to the EPR Hamiltonian (appearing in [18, Lemma 7] for example).

► **Lemma 3.** *For any n -qubit state ρ and $i \in [n]$,*

$$\sum_{j \neq i} \max(0, 2 \text{tr}(\rho \cdot E_{ij}) - 1) \leq 1.$$

As a consequence, $\{\max(0, 2 \text{tr}(\rho \cdot E_{ij}) - 1)\}_{i < j}$ always gives a feasible solution to the LP, implying that $\sum_{i < j} w_{ij} \max(0, 2 \text{tr}(\rho \cdot E_{ij}) - 1) \leq \text{LP}(w)$. This implies the upper bound

$$\lambda_{\max}(H) = \max_{\rho \geq 0, \text{tr}(\rho)=1} \text{tr}(\rho \cdot H) \leq \frac{\sum_{i < j} w_{ij} + \text{LP}(w)}{2} = \sum_{i < j} w_{ij} \tilde{E}_{ij}. \quad (1)$$

All the algorithms we present in this paper involve computing an optimal solution x to $\text{LP}(w)$, and applying a *rounding algorithm* to x to compute the description of a state ρ achieving energy

$$\text{tr}(\rho \cdot E_{ij}) \geq \alpha \cdot \tilde{E}_{ij} \quad (2)$$

on every edge $\{i, j\} \in \binom{[n]}{2}$ for some $\alpha > 0$. By Equation (1), we have

$$\text{tr}(\rho \cdot H) = \sum_{i < j} w_{ij} \cdot \text{tr}(\rho \cdot E_{ij}) \geq \alpha \cdot \sum_{i < j} w_{ij} \tilde{E}_{ij} \geq \alpha \cdot \lambda_{\max}(H),$$

so this results in an α -approximation algorithm.

Let us describe the rough plan for our presentation of this rounding algorithm. First, in Section 2.2, we describe how to use a rounding strategy used in the work of Lee and Parekh [20] to achieve $\alpha = 3/4$ in the special case that the interaction matrix w is bipartite, that is, it is the adjacency matrix of a bipartite weighted graph. Next, in Section 2.3 we give an improved rounding algorithm achieving $\alpha = \frac{1+\sqrt{5}}{4}$ for bipartite instances. Finally, in Section 2.4 we show how to achieve the same approximation ratio $\alpha = \frac{1+\sqrt{5}}{4}$ for general non-bipartite instances, proving Theorem 1.

2.2 A 3/4-approximation in the bipartite case

Here we focus on the case that w is the adjacency matrix of a weighted bipartite graph. For bipartite graphs, it was proved by Edmonds that the fractional matching LP is integral, i.e., its vertices are indicator vectors of matchings.

► **Lemma 4** ([10]). *For any weighted bipartite graph with adjacency matrix w , $\text{LP}(w) = w(M)$, where M is the maximum weight matching of the graph. That is, the optimal solution to $\text{LP}(w)$ is achieved by an integer vector $x_{ij} = \mathbf{1}_{\{\{i,j\} \in M\}}$.*

We can find such an optimal solution using an algorithm for maximum weighted matching. Let $U \subseteq [n]$ be the set of vertices that do not appear in the matching M . Consider the two states

$$\rho_{\text{prod}} = |0^n\rangle\langle 0^n|, \quad \rho_{\text{match}} = \left(\bigotimes_{\{i,j\} \in M} (|\text{EPR}\rangle\langle \text{EPR}|)_{i,j} \right) \otimes \left(\bigotimes_{i \in U} \frac{I_i}{2} \right).$$

The rounding algorithm will output a random choice between ρ_{prod} and ρ_{match} . In particular, we output the state $\rho = (1-p) \cdot \rho_{\text{prod}} + p \cdot \rho_{\text{match}}$ for some choice of $p \in [0, 1]$.

▷ **Claim 5.** The energy attained on edge $\{i, j\}$ is

$$\text{tr}(\rho \cdot E_{ij}) = \begin{cases} \frac{1}{2} + \frac{p}{2} & \text{if } \{i, j\} \in M, \\ \frac{1}{2} - \frac{p}{4} & \text{if } \{i, j\} \notin M. \end{cases}$$

On the other hand, the LP energy on edge $\{i, j\}$ is

$$\tilde{E}_{ij} = \frac{1 + x_{ij}}{2} = \begin{cases} 1 & \text{if } \{i, j\} \in M, \\ \frac{1}{2} & \text{if } \{i, j\} \notin M. \end{cases}$$

If we set $p = 1/2$, then one can check that for each edge $\{i, j\}$,

$$\text{tr}(\rho \cdot E_{ij}) = \frac{3}{4} \tilde{E}_{ij},$$

proving Equation (2) for $\alpha = \frac{3}{4}$.

2.3 An improvement in the bipartite case

Our improvement to this algorithm is simple to state – we interpolate between ρ_{prod} and ρ_{match} using quantum superposition rather than in probability. Concretely, let M be the maximum matching and U be the unmatched vertices as in Section 2.2. Define the tilted EPR state $|\text{EPR}_\theta\rangle := \sqrt{\theta}|00\rangle + \sqrt{1-\theta}|11\rangle$. We will output the state

$$\rho = \left(\bigotimes_{\{i,j\} \in M} (|\text{EPR}_\theta\rangle\langle \text{EPR}_\theta|)_{i,j} \right) \otimes \left(\bigotimes_{i \in U} (\theta|0\rangle\langle 0| + (1-\theta)|1\rangle\langle 1|)_i \right). \quad (3)$$

▷ **Claim 6.** The energy attained on edge $\{i, j\}$ is

$$\text{tr}(\rho \cdot E_{ij}) = \begin{cases} \frac{1}{2} + \sqrt{\theta(1-\theta)} = \frac{1}{2} + \gamma & \text{if } \{i, j\} \in M, \\ \frac{1}{2} - \theta(1-\theta) = \frac{1}{2} - \gamma^2 & \text{if } \{i, j\} \notin M, \end{cases}$$

where $\gamma = \sqrt{\theta(1-\theta)}$.

Comparing Claim 6 to Claim 5, one can readily see that this algorithm performs strictly better; for instance, set $\gamma = p/2$. Our new rounding scheme achieves strictly better energy on edges outside M and identical energy on edges inside M .

It remains to prove Claim 6, and then to analyze the approximation ratio of this rounding algorithm. We will repeatedly use the following simple properties of $|\text{EPR}_\theta\rangle$.

▷ **Claim 7.** Let $\gamma = \sqrt{\theta(1-\theta)}$. The following are true.

1. $|\langle \text{EPR} | \text{EPR}_\theta | \text{EPR} | \text{EPR}_\theta \rangle|^2 = \frac{1}{2} + \gamma$.
2. $\text{tr}_{[1]} |\text{EPR}_\theta\rangle\langle \text{EPR}_\theta| = \text{tr}_{[2]} |\text{EPR}_\theta\rangle\langle \text{EPR}_\theta| = \theta |0\rangle\langle 0| + (1-\theta) |1\rangle\langle 1|$.
3. $\langle \text{EPR} | (\theta |0\rangle\langle 0| + (1-\theta) |1\rangle\langle 1|)^{\otimes 2} | \text{EPR} \rangle = \frac{1}{2} - \gamma^2$.

Now, one can compute all the 2-qubit marginals:

$$\text{tr}_{[n]\setminus\{i,j\}}(\rho) = \begin{cases} |\text{EPR}_\theta\rangle\langle \text{EPR}_\theta| & \text{if } \{i,j\} \in M, \\ (\theta |0\rangle\langle 0| + (1-\theta) |1\rangle\langle 1|)^{\otimes 2} & \text{if } \{i,j\} \notin M, \end{cases}$$

where for the second case we used that the 1-qubit marginals are all equal to $\text{tr}_{[n]\setminus\{1\}}[|\text{EPR}_\theta\rangle\langle \text{EPR}_\theta|] = \theta |0\rangle\langle 0| + (1-\theta) |1\rangle\langle 1|$. By Claim 7, the energy achieved by each term $\{i,j\}$ is determined by

$$\langle \text{EPR} | \text{tr}_{[n]\setminus\{i,j\}}(\rho) | \text{EPR} \rangle = \begin{cases} \frac{1}{2} + \sqrt{\theta(1-\theta)} = \frac{1}{2} + \gamma & \text{if } \{i,j\} \in M, \\ \frac{1}{2} - \theta(1-\theta) = \frac{1}{2} - \gamma^2 & \text{if } \{i,j\} \notin M, \end{cases}$$

and Claim 6 follows immediately. Now let us analyze the approximation ratio. Similarly to Section 2.2, we have the LP energy

$$\tilde{E}_{ij} = \begin{cases} 1 & \text{if } \{i,j\} \in M, \\ \frac{1}{2} & \text{if } \{i,j\} \notin M. \end{cases} \quad (4)$$

Setting $\gamma = \frac{\sqrt{5}-1}{4}$, one can check using Equation (4) and Claim 6 that

$$\text{tr}(\rho \cdot E_{ij}) = \frac{1 + \sqrt{5}}{4} \cdot \tilde{E}_{ij}$$

for each edge $\{i,j\} \in \binom{[n]}{2}$. Thus, we have shown Equation (2) with $\alpha = \frac{1+\sqrt{5}}{4}$ as desired.

2.4 General Case

In the general non-bipartite case, we cannot apply Lemma 4; the fractional matching LP is not necessarily integral. Previous works proceeded by bounding the integrality gap of this LP, which is quite lossy. Our main idea is to take advantage of the fact that the fractional matching LP is *half-integral*.

► **Lemma 8** ([22, Theorem 7.5.1]). *For any weighted n -vertex graph with adjacency matrix w , there is a vertex-disjoint collection of edges $M \subset \binom{[n]}{2}$ and cycles $\mathcal{C} \subset 2^{\binom{[n]}{2}}$ such that $\text{LP}(w) = w(M) + \frac{1}{2} \sum_{C \in \mathcal{C}} w(C)$. That is, the optimal solution to $\text{LP}(w)$ is achieved by the half-integer vector $x_{ij} = \mathbf{1}_{\{\{i,j\} \in M\}} + \frac{1}{2} \sum_{C \in \mathcal{C}} \mathbf{1}_{\{\{i,j\} \in C\}}$.*

In particular, (e.g. using the algorithm of Anstee [2]), one can efficiently find such a solution x , i.e. a vertex-disjoint collection of edges $M \subset \binom{[n]}{2}$ and odd length cycles \mathcal{C} such that the LP energies can be written as

$$\tilde{E}_{ij} = \frac{1 + x_{ij}}{2} = \begin{cases} 1 & \text{if } \{i,j\} \in M, \\ \frac{3}{4} & \text{if } \{i,j\} \in C \text{ for some } C \in \mathcal{C}, \\ \frac{1}{2} & \text{otherwise.} \end{cases} \quad (5)$$

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Let U be the set of vertices absent from M and \mathcal{C} . The algorithm in the bipartite case (Equation (3)) already suggests what quantum state we will output on the qubits involved in M and U . On the qubits in C for some odd cycle $C \in \mathcal{C}$ of length k , we will output a high energy state for the EPR Hamiltonian on the length k cycle, i.e. $H_{\text{cycle}} = \sum_{i \in [k]} E_{i, i+1 \pmod k}$, subject to the constraint that all 1-qubit marginals are equal to $\theta |0\rangle\langle 0| + (1 - \theta) |1\rangle\langle 1|$. The following lemma (which we prove in Section A) shows that there is a way to achieve sufficiently large energy on the cycle edges.

► **Lemma 9.** *For any integer k , there is an efficient algorithm to compute the description of a k -qubit state ρ_k satisfying the following, where $\gamma = \frac{\sqrt{5}-1}{4}$ and $\theta \geq 1/2$ is the solution to $\sqrt{\theta(1-\theta)} = \gamma$.*

1. For all $i \in [k]$, $\text{tr}(\rho_k \cdot E_{i, i+1 \pmod k}) > \frac{3}{4} \cdot \frac{1+\sqrt{5}}{4}$.
2. For all $i \in [k]$, the 1-qubit marginal $\text{tr}_{[k]-i}[\rho_k]$ equals $\theta |0\rangle\langle 0| + (1 - \theta) |1\rangle\langle 1|$.
3. For all $i, j \in [k]$, $\text{tr}(\rho_k \cdot E_{ij}) > \frac{1}{2} \cdot \frac{1+\sqrt{5}}{4}$.

► **Remark 10.** The main idea behind the proof is that Items 1–3 are all linear constraints in the positive semidefinite variable ρ_k , and hence the Lemma reduces to solving a semidefinite program of size $2^{\mathcal{O}(k)}$. This can be verified numerically for k small enough. When k is large, we instead choose ρ_k to be a tensor product of states on a disjoint collection of short paths; here the states on short paths are again found by numerically solving an appropriate semidefinite program.

The bounds in Lemma 9 are not tight – our numerical proof already shows that Items 1–3 can be simultaneously improved. However, for ease of exposition we have chosen to write the weakest bounds that suffice to attain the required approximation ratio.

Our algorithm will output the state

$$\rho = \left(\bigotimes_{C \in \mathcal{C}} (\rho_{|C|})_{V(C)} \right) \otimes \left(\bigotimes_{\{i, j\} \in M} (|\text{EPR}_\theta\rangle\langle \text{EPR}_\theta|)_{i, j} \right) \otimes \left(\bigotimes_{i \in U} (\theta |0\rangle\langle 0| + (1 - \theta) |1\rangle\langle 1|)_i \right), \quad (6)$$

where $V(C) \subseteq [n]$ is the set of qubits in the cycle C and $\rho_{|C|}$ is the state guaranteed by Lemma 9. Similarly to Section 2.3, we set $\gamma = \frac{\sqrt{5}-1}{4}$ and $\theta \geq 1/2$ such that $\sqrt{\theta(1-\theta)} = \gamma$. Let us analyze the energy achieved by this algorithm. We have

$$\text{tr}(\rho \cdot E_{ij}) \geq \begin{cases} \frac{1+\sqrt{5}}{4} & \text{if } \{i, j\} \in M, & (\text{Claim 6}) \\ \frac{3}{4} \cdot \frac{1+\sqrt{5}}{4} & \text{if } \{i, j\} \in C \text{ for some } C \in \mathcal{C}, & (\text{Lemma 9, Item 1}) \\ \frac{1}{2} \cdot \frac{1+\sqrt{5}}{4} & \text{otherwise.} & (\text{1-qubit marginals, Lemma 9, Item 3}) \end{cases}$$

To elaborate on the last case, we note that it must be that either qubits i and j are nonadjacent vertices in the *same* cycle $C \in \mathcal{C}$, or they are in tensor product. If the former is true, we use the guarantee of Lemma 9, Item 3. Otherwise, we use the fact that all the 1-qubit marginals are equal to $\theta |0\rangle\langle 0| + (1 - \theta) |1\rangle\langle 1|$ along with the calculations from Section 2.3 to conclude that the energy is $\frac{1}{2} - \gamma^2 = \frac{1+\sqrt{5}}{8}$.

Comparing with Equation (5), we immediately get that for every edge $\{i, j\} \in \binom{[n]}{2}$,

$$\text{tr}(\rho \cdot E_{ij}) \geq \frac{1 + \sqrt{5}}{4} \tilde{E}_{ij},$$

proving Equation (2) with $\alpha = \frac{1+\sqrt{5}}{4}$. As a result, we obtain an approximation algorithm for the EPR Hamiltonian with approximation ratio $\frac{1+\sqrt{5}}{4}$, proving Theorem 1.

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A Proof of Lemma 9

For the reader’s convenience we restate Lemma 9 below. The code for verifying the numerical claims made in the below proof is available at <https://github.com/anshnagda/EPR-algorithm>.

► **Lemma 11** (Restatement of Lemma 9). *For any integer k , there is an efficient algorithm to compute the description of a k -qubit state ρ_k satisfying the following, where $\gamma = \frac{\sqrt{5}-1}{4}$ and $\theta \geq 1/2$ is the solution to $\sqrt{\theta(1-\theta)} = \gamma$.*

1. For all $i \in [k]$, $\text{tr}(\rho_k \cdot E_{i,i+1(\text{mod } k)}) > \frac{3}{4} \cdot \frac{1+\sqrt{5}}{4}$.
2. For all $i \in [k]$, the 1-qubit marginal $\text{tr}_{[k]-i}[\rho_k]$ equals $\theta |0\rangle\langle 0| + (1-\theta) |1\rangle\langle 1|$.
3. For all $i, j \in [k]$, $\text{tr}(\rho_k \cdot E_{ij}) > \frac{1}{2} \cdot \frac{1+\sqrt{5}}{4}$.

Proof. For $k \leq 5$, we numerically verify the claim by explicitly solving a semidefinite program.

Similarly, one can verify by solving a semidefinite program that there exists a 5-qubit state ψ satisfying the following:

1. $\frac{1}{4} \cdot \sum_{i \in [4]} \text{tr}(E_{i,i+1} \cdot \psi) \geq 0.668$.
2. For all $i, j \in [5]$, $\text{tr}(E_{ij} \cdot \psi) > \frac{1}{2} \cdot \frac{1+\sqrt{5}}{4}$.
3. For all $i \in [5]$, the 1-qubit marginal $\text{tr}_{[5]-i}[\psi]$ equals $\theta |0\rangle\langle 0| + (1-\theta) |1\rangle\langle 1|$.

Now assume $k \geq 7$. Define the state

$$\rho'_k = |\text{EPR}_\theta\rangle\langle \text{EPR}_\theta|^{\otimes \frac{k-5}{2}} \otimes \psi.$$

Let Shift_i be the unitary that shifts qubits in the k -cycle i spots. We will set ρ_k to be the shift-invariant state

$$\rho_k = \mathbb{E}_{i \sim [k]} \left[\text{Shift}_i \cdot \rho'_k \cdot \text{Shift}_i^\dagger \right].$$

We will verify that ρ_k satisfies the three requirements.

1. Let $i \in [k]$. We can write the energy $\text{tr}(\rho_k \cdot E_{i,i+1(\text{mod } k)})$ as the average energy of a random edge $\{j, j+1(\text{mod } k)\}$ under ρ'_k . By definition of ρ'_k , one can compute

$$\text{tr}(\rho'_k \cdot E_{j,j+1(\text{mod } k)}) \geq \begin{cases} \frac{1+\sqrt{5}}{4} & j \leq k-5 \text{ odd,} \\ \frac{1+\sqrt{5}}{8} & j \leq k-5 \text{ even or } j = k. \end{cases}$$

For the cases $k-5 < j < k$, the assumption on ψ allows us to bound the energy as

$$\sum_{k-5 < j < k} \text{tr}(\rho'_k \cdot E_{j,j+1(\text{mod } k)}) \geq 4 \cdot 0.668.$$

Therefore

$$\text{tr}(\rho_k \cdot E_{i,i+1(\text{mod } k)}) = \frac{\frac{k-5}{2} \cdot \frac{1+\sqrt{5}}{4} + \frac{k-5}{2} \cdot \frac{1+\sqrt{5}}{8} + 4 \cdot 0.668 + \frac{1+\sqrt{5}}{8}}{k}.$$

One can verify that $4 \cdot 0.668 + \frac{1+\sqrt{5}}{8} > 5 \cdot \frac{3}{4} \cdot \frac{1+\sqrt{5}}{4}$, implying

$$\text{tr}(\rho \cdot E_{i,i+1(\text{mod } k)}) > \frac{(k-5) \cdot \frac{3}{4} \cdot \frac{1+\sqrt{5}}{4} + 5 \cdot \frac{3}{4} \cdot \frac{1+\sqrt{5}}{4}}{k} = \frac{3}{4} \cdot \frac{1+\sqrt{5}}{4}.$$

2. It suffices to prove that the 1-qubit marginals of ρ'_k are equal to $\theta |0\rangle\langle 0| + (1-\theta) |1\rangle\langle 1|$. For qubits $i \leq k-5$, this follows from Claim 7, and for $i > k-4$, this follows by definition of ψ .
3. Let $i \neq j$. It suffices to prove $\text{tr}(\rho'_k \cdot E_{ij}) > \frac{1}{2} \cdot \frac{1+\sqrt{5}}{4}$ the same for ρ'_k . We consider three cases.
 - If $j = i+1$ for some odd $i \leq k-5$, this is implied by Item 1.
 - If $k-5 < i, j \leq k$, this is implied by the definition of ψ .
 - Otherwise, the 2-qubit marginal $\text{tr}_{[n] \setminus \{i,j\}}(\rho'_k)$ equals $(\theta |0\rangle\langle 0| + (1-\theta) |1\rangle\langle 1|)^{\otimes 2}$, and this is implied by Claim 7. ◀