Product-State Approximation Algorithms for the Transverse Field Ising Model

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Abstract

We study classical polynomial-time approximation algorithms for the transverse field Ising model (TFIM), allowing a mixture of ferromagnetic and antiferromagnetic interactions between pairs of qubits, alongside transverse field terms with arbitrary non-negative weights.

In this work, we first prove a second-order conic inequality based on the anticommutation property of the two competing terms (Ising Z_iZ_j vs. field X_i terms), and we use this inequality to strengthen the basic SDP relaxation of the problem. By producing two competing rounded product state solutions and taking the better of the two we achieve an approximation ratio $\gamma \approx 0.7860$. A further improvement by non-uniform interpolation achieves a ratio $\gamma \approx 0.82197$. Finally, we give an explicit purely antiferromagnetic TFIM instance on three qubits for which every product state achieves at most $169/180 \approx 0.9389$ of the true optimum, yielding an upper bound for all algorithms producing product state approximations, even in the purely antiferromagnetic case.

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1 Introduction

Local Hamiltonians are operators associated with the total energy of quantum many-body systems and are represented by Hermitian matrices. Even though general Hamiltonians can have exponentially large descriptions with respect to the number of interacting particles, local Hamiltonians can be succinctly represented as the summation of only the non-trivial locally interacting terms, which are usually very small (2 or 3).

The *Local Hamiltonian problem* asks to determine whether the *ground state energy* (associated with the smallest eigenvalue of the operator) of a given local Hamiltonian is below a certain threshold α or above a different threshold β, with a promise that one of these two conditions holds. This problem is the quantum analogue of classical constraint satisfaction problems [15]. In a seminal work [28] Kitaev showed that computing the ground state energy of such Hamiltonians is a **QMA**-hard problem [7], even when the interactions are restricted in a one-dimensional line and the dimension of each particle is bounded by 12 [25, 1, 2]. This formalizes our belief that such problems remain intractable even for fault-tolerant quantum computers (if and when they might be built).

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In recent years, the study of Local Hamiltonians has also attracted growing interest within the computer science community. Given the fundamental importance and computational intractability of the problem, research efforts have focused on finding *approximation algorithms*: efficient algorithms designed to estimate the ground-state energy by producing low-energy states that approximate the true ground state within provable performance guarantees [8, 11, 16, 17, 20, 35, 36, 3, 27, 34, 40, 42, 29, 13, 19, 6, 22, 24, 4]. These algorithms typically output product states or states that can be efficiently represented on a classical device, such as Matrix Product States. Although the "ansatzes" from which these states are drawn are not fully general, MPS are frequently relevant in practice, for example in the efficient simulation of material properties in quantum chemistry.

The Transverse Field Ising model (TFIM) is a well-known and well-studied quantum spin system consisting of competing *Ising* interactions and *transverse fields*. An instance consisting of n interacting particles (qubits) can be represented by a simple, undirected graph $G = (V, E)$ with vertex set V, one for each particle, and edge set E, one for each pair of interacting particles. The TFIM Hamiltonian is defined as

$$H_{\text{TFIM}} = \sum_{\{i,j\}\in E} w_{ij} J_{ij} Z_i Z_j - \sum_{i\in V} h_i X_i, \qquad J_{ij} \in \{-1, +1\}, w_{ij}, h_i \geq 0. \tag{1}$$

where X_i, Z_i are Pauli operators on qubit i, J_{ij} are arbitrarily signed couplings and h_i are the single-qubit transverse field strengths.

This paper studies *multiplicative* approximation algorithms, which are subtle in quantum Hamiltonian complexity because, for instance, the ground state energy of the Hamiltonian as written in (1) could be negative or even zero. More generally, adding a constant multiple of the identity changes multiplicative approximability even though it does not change the ground state. This is the same classical phenomenon behind "Ising energy" versus "Max-Cut" objectives, and is explicitly discussed in the quantum setting (i.e., Gharibian-Parekh [17] for the Heisenberg model). Consequently, we fix an equivalent maximization version of the problem in which the Hamiltonian is a weighted sum of local *projections* (taking values between 0 and 1), and we approximate its maximum eigenvalue.

Given the equivalent formulation of the TFIM problem, we design classical polynomial-time algorithms that return explicit *product states* (unentangled states) achieving a guaranteed fraction of the true, and possibly highly entangled, quantum optimum. Product states, the canonical output for most of the classical algorithms, form a natural restricted ansatz (mean-field) and are algorithmically attractive due to efficient description and evaluation. Indeed, a product state can be described with polynomially many bits (in the input instance size), as opposed to general (entangled) quantum states which require exponentially many classical bits to describe. In some cases where the specific geometry of the underlying Hamiltonian term allows it, like Quantum Max Cut, algorithms are known that output mildly entangled states, see Remark 2.

The central question we address thus is: *how well can one efficiently approximate the ground state (energy) of TFIM instances?* We note that this was left as an open question in [17] where the authors explicitly ask for the approximability properties of "intermediate" Hamiltonian models, such as TFIM.

Our Contributions. We give two constant-factor approximation algorithms and one product-state upper bound.

1. We introduce an SDP relaxation which we crucially strengthen by *second-order conic* (SOC) inequalities capturing the local incompatibility (anticommutation) between the X_i and Z_iZ_j observables. We define two rounded product-state candidate solutions

and return the better of the two: a standard hyperplane rounding focusing on the ZZ-interactions, and a second rounding that uses to the full extent the SOC-SDP X values but crucially uses the SOC tradeoff in order to lower bound the ZZ-correlation that may remain given the SDP's X mass. By a balancing analysis this yields an approximation ratio of ≈ 0.7860.

2. Our second algorithm performs interpolation in a non-uniform way on the x variables corresponding to the X observables obtained by the SOC-SDP: instead of fully trusting the SDP solution values for the x variables, as in the previous solution, we scale them in a non-uniform way. This might "tilt" the solution more towards the ZZ terms. By bounding each term's contributions we obtained an improved 0.82197-approximation algorithm.
3. We construct a simple example with an explicit product-state optimality gap of (169/180), demonstrating that no algorithm that outputs product states can achieve better than $169/180 \approx 0.9388$-approximation ratio against the true optimum.

All guarantees hold for *arbitrary sign patterns* $J_{ij} \in \{\pm 1\}$ (including frustrated spin glasses) and weighted constraints. Also these approximation guarantees can be compared to the UGC-hardness bound of $\alpha_{\mathrm{GW}} \approx 0.8786$ inherited from classical MaxCut. We also note that the "baseline" algorithm that (i) optimizes in the X direction (the $|+\rangle$ state), (ii) independently apply the hyperplane rounding to extract a ZZ solution, and finally taking the maximum of the two previous solutions achieves 0.71-approximation guarantee.

▶ Remark 1. Our relaxation and rounding scheme has an "integrality gap" already on the antiferromagnetic complete graphs with uniform field strengths $h_i = g$. The relevant quantity is the *advantage* over the trivial baseline $S/2$ where S is the sum of all edge weights and all vertex field strengths. The SOC-SDP optimum can be assumed, by symmetry, to have $x_i = x$ and $c_{ij} = c$ for all field and all Ising terms respectively. Its optimal value can be thus represented in closed form as $\frac{1}{2}\sqrt{m^2 + (gn)^2}$, m being the number of Ising terms (edges). The advantage gained by the optimal product state is $\frac{m}{2}\max_x(1 - x^2 + \frac{gn}{m}x)$. Comparing and optimizing over g, gives us the ratio $\frac{\sqrt{3}}{2} \approx 0.866025$.

▶ Remark 2. In the last couple of years, a lot of attention has been given to the Heisenberg (aka Quantum Max Cut) Hamiltonian. For this, the interest has been shifted from product-states to more sophisticated entangling and QMC-specific *ansatzes* [27, 29, 19, 5, 4]. In QMC the interactions are purely 2-local and the algorithmic leverage comes from entangling some of the qubits in a matching-like fashion. Monogamy of entanglement inequalities allow then to compare these entangled edges directly to the product state SDP solution, giving higher guarantees. However, the nature of TFIM structure and geometry are very different. Here, the obstruction is not how to entangle neighboring qubits, but the incompatibility of the two observables. In particular, each field term X_i is simultaneously incompatible with *all* incident edge terms Z_iZ_j. This is precisely the utility of our underlying SOC inequality. It is not clear at all what a good entangling strategy would be, and, even if we had one, how would we relate it to the SOC-SDP. We leave this as a very interesting open direction.

Scope relative to prior work. TFIM is one of the canonical and extensively studied quantum spin systems, both in quantum many-body physics and in quantum computation. On the physical side, TFIM exhibits quantum phase transition as the 1D TFIM (interacting particles are assembled on the line with closest neighbor interaction) is exactly solvable and exhibits zero-temperature order-disorder transition [37], but higher dimensional instances of TFIM are studied extensively for quantum dynamics and Kibble-Zurek phenomena [39]. On the other hand, the time-dependent TFIM is used in quantum annealing hardware and algorithmic processes [23, 14].

On the complexity side, Bravyi and Hastings [12] showed that estimating the ground state energy of TFIM on degree-3 graphs is a complete problem for the complexity class **StoqMA**. We recall that **MA** $\subseteq$ **StoqMA** $\subseteq$ **QMA** and that **StoqMA** is believed to be strictly smaller than **QMA** [9]. Bravyi and Gosset [10] give randomized approximation schemes for the *partition function* (hence additive free-energy/ground-energy estimates) for certain stoquastic models including antiferromagnetic ($J_{ij} \geq 0$) TFIM after a basis change. Our approach, on the other hand, works for arbitrary sign patterns and weights. We note that computing the partition function allows one also to solve the corresponding local Hamiltonian. We also note that [6] gives a PTAS for the more general quantum Ising model on the restricted class of *bounded degree planar graphs*, for which computing the optimum is **QMA**-hard [32]. Such additive schemes do not address worst-case *multiplicative* approximation of the normalized Hamiltonian, nor they seem to extent to arbitrary signed/frustrated couplings. In contrast, our results not only apply to signed instances but also provide explicitly constructed product states with guaranteed multiplicative factor with respect to the true quantum optimum. Works on the quantum Heisenberg/Quantum MaxCut Hamiltonians study different local terms. For more general traceless 2-local Hamiltonians, there is a well-known constant lower bound of 1/9 for product states [30] as well as $\mathcal{O}(\log(n))$-approximation algorithms [11]. While the algorithms proposed in [11] deal with a more general case compared to our approach, they achieve non-constant approximation ratios. We also note that Parekh, Rayudu, and Thompson [33] have also studied quantum generalizations of the Vertex Cover problem and introduced a quantum local ratio method. In addition to their *Transverse* Vertex Cover problem they have also applied the method to a local Hamiltonian formulation they called *Transverse Prize Collecting* Vertex Cover which is related to the antiferromagnetic transverse Ising models after a PSD rearrangement, but their approximability results are not directly comparable to our SDP multiplicative approximations since they concern a different minimization objective function.

2 The Model and its relaxation

On one qubit, let

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \qquad \mathbb{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

On n qubits, X_i denotes X acting on qubit i tensored with identity on all the others; similarly for Z_i. The subscript is omitted when there is no ambiguity. Pauli operators satisfy $X_i^2 = Z_i^2 = \mathbb{I}$, and they anticommute when acting on the same qubit $X_iZ_i = -Z_iX_i$, while they commute when acting on different qubits. When we write, for example, Z_iZ_j we mean $Z_i \otimes Z_j$ but for convenience we drop the tensor product operator.

A (mixed) quantum state on n qubits is a density matrix $\rho \succeq 0$ with $\mathrm{Tr}(\rho) = 1$. For a Hermitian observable A, its expectation value is denoted $\langle A \rangle_\rho = \mathrm{Tr}(\rho A)$. A *product state* is a state that can be written as $\rho = \rho_1 \otimes \cdots \otimes \rho_n$. Any state that cannot be written in the previous format is called an *entangled state*. For an n-qubit system, where each qubit is living in $\mathbb{C}^2$ (or, more generally, in $\mathbb{C}^d$ for qudit systems), any quantum state $|\psi\rangle$ lives in $\mathbb{C}^{2^n}$ ($\mathbb{C}^{d^n}$ for qudits) i.e., it is an exponentially with respect to n long vector. But, in contrast, product states $\rho = \rho_1 \otimes \cdots \otimes \rho_n \in (\mathbb{C}^2)^{\otimes n}$ which can be described with polynomially many terms. Any single-qubit state can be written in the Bloch form $\rho_i = \frac{1}{2}(\mathbb{I} + x_iX + y_iY + z_iZ)$, such that $x_i^2 + y_i^2 + z_i^2 \leq 1$. We note that $\langle X_i \rangle_{\rho_i} = x_i$ and $\langle Z_i \rangle_{\rho_i} = z_i$.

2.1 Formulating the approximation problem

A fundamental computational task is to approximate the ground-state energy $\lambda_{\min}(H_{\text{TFIM}})$ and to output a quantum state (in our case, a *product state*) whose energy is close to optimum (ground state). For classical approximation algorithms, however, the "usual" multiplicative approximation ratio for minimization is not well suited for quantum Hamiltonians because the ground energy can be negative, or even zero. To obtain a robust notion of approximation we transform our H_{TFIM} to an equivalent *maximization* formulation built from positive semidefinite (PSD) "constraint" operators. This affine shift does not change the physics of the model, it only transforms the Hamiltonian to one where the approximation mechanics make sense. The idea is to replace each local term by a PSD operator that rewards the *locally energy-minimizing* eigenspace, so that the global objective becomes a sum of nonnegative constraint values. This provides a natural scale for multiplicative approximation guarantees.

For an edge $\{i,j\} \in E$, the operator $J_{ij}Z_iZ_j$ has eigenvalues $+1/-1$. The contribution of this edge to (1) is minimized when $J_{ij}Z_iZ_j = -1$. This can happen in two ways: either $J_{ij} = +1$ in which case the corresponding vertices would like to be *anti*-aligned (an "antiferromagnetic" interaction), or $J_{ij} = -1$ in which case i and j would like to be aligned in the z-direction (a "ferromagnetic" interaction). We define the PSD projector onto this minimizing eigenspace: $\Pi^Z_{ij} = \frac{1}{2}(\mathbb{I} - J_{ij}Z_iZ_j)$. This operator has eigenvalues $\{0,1\}$ and equals 1 exactly when the edge is "satisfied" in the energy-minimizing sense.

Similarly for the field "constraints", for a vertex $i \in V$ the single-qubit operator $-h_iX_i$ is minimized when $X_i = +1$ (the $|+\rangle$ eigenstate of X). We define the PSD projector onto this minimizing eigenspace: $\Pi^X_i = \frac{1}{2}(\mathbb{I} + X_i)$. Again Π^X_i has eigenvalues $\{0,1\}$.

We can now define the equivalent transformed Hamiltonian by summing these PSD constraints with the same nonnegative weights as in the TFIM:

$$H_{\text{TFIM}'} = \sum_{\{i,j\}\in E} w_{ij}\Pi^Z_{ij} + \sum_{i\in V} h_i\,\Pi^X_i. \tag{2}$$

By construction we have that $H_{\text{TFIM}'} \succeq 0$ and that $\langle\psi|H_{\text{TFIM}'}|\psi\rangle$ is the energy of the state $|\psi\rangle$. By expanding (2) we immediately see that maximizing $H_{\text{TFIM}'}$ is exactly equivalent to minimizing H_{TFIM}, up to an affine shift. Indeed,

$$H_{\text{TFIM}'} \;=\; \sum_{\{i,j\}\in E} w_{ij}\Pi^Z_{ij} + \sum_{i\in V} h_i\,\Pi^X_i = \frac{1}{2}\underbrace{\Big(\sum_{\{i,j\}\in E} w_{ij} + \sum_{i\in V} h_i\Big)}_{S}\mathbb{I} - \frac{1}{2}H_{\text{TFIM}}.$$

Taking maximum eigenvalues gives

$$\lambda_{\max}\big(H_{\text{TFIM}'}\big) = \frac{1}{2}S - \frac{1}{2}\lambda_{\min}\big(H_{\text{TFIM}}\big) \iff \lambda_{\min}\big(H_{\text{TFIM}}\big) = S - 2\lambda_{\max}\big(H_{\text{TFIM}'}\big).$$

Moreover, H_{TFIM} and $H_{\text{TFIM}'}$ have the same eigenvectors, so any state that *approximates* (2) immediately yields an approximate solution for (1).

▶ Remark 3. In the case where all $h_i = 0$ and all $J_{ij} = 1$ we have that $\lambda_{\max}(H_{\text{TFIM}'}) = \textsc{MaxCut}(G)$. Since the latter is known to be UGC-hard to approximate with approximation ratio better than $\alpha_{\text{GW}} \approx 0.8786$ [26], we have the same inapproximability result for $\lambda_{\max}(H_{\text{TFIM}'})$.

3 A SOC-SDP relaxation upper-bounding the true quantum optimum

Before we go to the algorithms, we first provide the key geometric lemma behind our relaxation and then we define the relaxation.

The anticommutation tradeoff inequality. The key local geometric constraint comes from anticommutation. Intuitively, by Heisenberg's uncertainty principle, a single qubit cannot simultaneously have large X and large Z polarization. We translate our intuition into a quantitative tradeoff between $\langle X_i \rangle$ and any incident correlation $\langle Z_i Z_j \rangle$.

▶ **Lemma 4.** *Let A, B be any Hermitian operators with $A^2 = B^2 = \mathbb{I}$ and $AB = -BA$, i.e., A and B anticommute. Then for any state ρ we have that $\langle A \rangle_\rho^2 + \langle B \rangle_\rho^2 \leq 1$.*

Proof. Let $a = \langle A \rangle_\rho = \mathrm{Tr}[\rho A]$ and $b = \langle B \rangle_\rho = \mathrm{Tr}[\rho B]$, and define $M = aA + bB$. Using $A^2 = B^2 = \mathbb{I}$ and $AB = -BA$, we get

$$M^2 = a^2 A^2 + b^2 B^2 + ab(AB + BA) = (a^2 + b^2)\mathbb{I},$$

hence $\|M\| = \sqrt{a^2 + b^2}$. On the other hand, because of the linearity of the trace $\mathrm{Tr}[\rho M] = a\,\mathrm{Tr}[\rho A] + b\,\mathrm{Tr}[\rho B] = a^2 + b^2$. Since $|\,\mathrm{Tr}[\rho M]| \leq \|M\|_{\mathrm{op}}$ for Hermitian M, we obtain $a^2 + b^2 \leq \sqrt{a^2 + b^2}$ i.e., $a^2 + b^2 \leq 1$. ◀

By choosing $A = X_i$ and $B = Z_i Z_j$ we get that $\langle X \rangle_\rho^2 + \langle Z_i Z_j \rangle_\rho^2 \leq 1$.

▶ Remark 5. We note that by using the same assumptions of Lemma 4, the same inequality can be derived using the second level of the non-commutative (quantum) Lasserre hierarchy [31, 38] and of levels of moment/SoS hierarchies for mutually anti-commuting terms, see [21]. In our setting we do not need the full power of nc-Lasserre, enhancing the natural SDP with these inequalities is enough for our purposes.

▶ Remark 6. We note that, although physically quite natural, without this anticommutation inequality the relaxation would not be able to enforce the basic incompatibility between the X and ZZ terms. In particular, nothing would forbid the SDP to assign $x_i = c_{ij} = 1$ but this would have absolutely no physical meaning since, because the corresponding observables anticommute, there is no quantum state realizing those marginals. The inequality not only rules this out, but also let us turn the SDP upper bound to a good, actually realizable, quantum state.

3.1 The relaxation

We now define a convex relaxation that upper-bounds the *true quantum optimum* $\mathrm{OPT} = \lambda_{\max}(H_{\mathrm{TFIM}'})$. The relaxation uses variables for (i) single-qubit X-expectations $x_i \approx \langle X_i \rangle$, and (ii) pairwise ZZ correlations $c_{ij} \approx \langle Z_i Z_j \rangle$. Lemma 4 yields the SOC constraints relation between x_i and c_{ij} on each edge incident to i.

Recalling from Section 2 our projector "constraint" operators, for each edge $\{i, j\}$ we define for convenience the signed variable $t_{ij} = -J_{ij} c_{ij}$, so that the (relaxed) edge constraint value is exactly $(1 + t_{ij})/2$, matching $\mathrm{Tr}[\Pi_{ij}^Z \rho]$.

▶ **Definition 7** (SOC-SDP relaxation)**.** *Let $n = |V|$. The relaxation has variables $x_i \in [-1, 1]$ and a matrix $C = (c_{ij})$ with $c_{ii} = 1$. Let $u_1, \ldots, u_n$ be unit vectors such that $c_{ij} = \langle u_i, u_j \rangle$, and define $t_{ij} := -J_{ij} c_{ij} \in [-1, 1]$. Maximize*

$$\mathrm{SDP} = \sum_{\{i,j\} \in E} w_{ij} \frac{1 + t_{ij}}{2} + \sum_{i \in V} h_i \frac{1 + x_i}{2} = \sum_{\{i,j\} \in E} \mathrm{SDP}_E[i, j] + \sum_{i \in V} \mathrm{SDP}_X[i] \tag{3}$$

subject to:

$$C = (C_{ij}) = (c_{ij}) \succeq 0, \tag{4}$$
$$\langle u_i, u_i \rangle = 1 \qquad \forall i \in V, \tag{5}$$
$$x_i \in [-1, 1] \qquad \forall i \in V, \tag{6}$$
$$x_i^2 + c_{ij}^2 \leq 1, \quad x_j^2 + c_{ij}^2 \leq 1 \qquad \forall \{i, j\} \in E. \tag{7}$$

The next lemma states that every quantum state induces feasible moments for the SOC-SDP with same objective function value i.e., the SOC-SDP is an upper bound on the true OPT even for arbitrary signed/frustrated patterns $J_{ij} \in \{\pm 1\}$.

▶ **Lemma 8.** *For every state ρ on n qubits, there exists a feasible solution to Definition 7 with objective value exactly* $\mathrm{Tr}[H_{\mathrm{TFIM}'}\rho]$. *Thus,* $\mathrm{SDP} \geq \mathrm{OPT} = \lambda_{\max}(H_{\mathrm{TFIM}'})$.

Proof. Let us fix an arbitrary quantum state ρ and let us define

$$x_i := \mathrm{Tr}[\rho X_i], \qquad c_{ij} := \mathrm{Tr}[\rho Z_i Z_j].$$

Since Pauli operators have operator norm 1, we have $|x_i| \leq 1$ and $|c_{ij}| \leq 1$.

PSD constraints. Let $C = (c_{ij})$ with $c_{ii} = 1$. For any $b \in \mathbb{R}^n$,

$$b^\top C b = \sum_{i,j} b_i b_j \ \mathrm{Tr}[\rho Z_i Z_j] = \mathrm{Tr}\left[\rho \left(\sum_i b_i Z_i\right)^2\right] \geq 0,$$

so $C \succeq 0$ and admits a Gram representation $c_{ij} = \langle u_i, u_j \rangle$ with $\|u_i\| = 1$.

SOC constraints. Fix an edge $\{i, j\} \in E$. Let $A = X_i$ and $B = Z_i Z_j$. Then $A^2 = B^2 = \mathbb{I}$ and $AB = -BA$. By Lemma 4,

$$\mathrm{Tr}[\rho X_i]^2 + \mathrm{Tr}[\rho Z_i Z_j]^2 \leq 1 \quad \Longleftrightarrow \quad x_i^2 + c_{ij}^2 \leq 1.$$

The same argument with X_j gives $x_j^2 + c_{ij}^2 \leq 1$.

Objective function value. Using $\Pi_{ij}^Z = \frac{1}{2}(\mathbb{I} - J_{ij} Z_i Z_j)$, $\Pi_i^X = \frac{1}{2}(\mathbb{I} + X_i)$ and linearity of trace:

$$\mathrm{Tr}[\Pi_{ij}^Z \rho] = \frac{1 - J_{ij}\,\mathrm{Tr}[\rho Z_i Z_j]}{2} = \frac{1 + (-J_{ij} c_{ij})}{2} = \frac{1 + t_{ij}}{2}, \quad \mathrm{Tr}[\Pi_i^X \rho] = \frac{1 + \mathrm{Tr}[\rho X_i]}{2} = \frac{1 + x_i}{2}.$$

Therefore the SOC-SDP objective equals $\mathrm{Tr}[H_{\mathrm{TFIM}'}\rho]$. Taking ρ to be an optimal eigenstate (ground state) for OPT yields $\mathrm{SDP} \geq \mathrm{OPT}$. ◀

In the analysis below, we solve the SOC-SDP relaxation up to some arbitrary precision $\epsilon \geq 0$ to obtain a feasible solution consisting of vectors x_i and a matrix $(C)_{ij}$ such that $c_{ij} = \langle u_i, u_j \rangle$. We denote by SDP the objective function value obtained (over the instance we are solving) and we further decompose SDP into the edge Ising terms and the field terms:

$$\mathrm{SDP} = \mathrm{SDP}_E + \mathrm{SDP}_X = \sum_{\{i,j\} \in E} \mathrm{SDP}_E[i, j] + \sum_{i \in V} \mathrm{SDP}_X[i].$$

4 A 0.786 approximation algorithm based on SOC-SDP

Our algorithm computes two randomized product-state candidates from the *same* SOC-SDP solution and returns the better one. The point of having two candidates is that different instances can be edge-dominated or field-dominated:

Candidate A (pure-ZZ solution): ignores the SDP x_i values and uses a GW style hyperplane rounding [18] on the edge constraints Z_iZ_j. This gives us a strong approximation guarantee on edges but only a trivial factor $1/2$ on the fields.

Candidate B (X, ZZ mixed solution): this solution matches the SDP field marginals exactly (hence achieves factor 1 on field constraints) and uses the remaining budget (if any) according to Lemma 4 in order to round the edge constraints.

4.1 A pure Z solution

Algorithm A, given some TFIM input instance for the transformed hamiltonian $H_{\mathrm{TFIM}'}$, solves the corresponding SOC-SDP to obtain a feasible solution, then ignores the x_i variables and uses a pure ZZ-basis rounding.

Algorithm A Pure ZZ solution.

Input: Unit vectors u_i from the SOC-SDP solution.

1. Sample $g \sim N(0, \mathbb{I})$.
2. Set $s_i = \mathrm{sign}(\langle g, u_i\rangle)$ for all i.
3. Output the product state $\rho = \bigotimes_i \rho_i$ where

$$\rho_i := \frac{1}{2}\Big(\mathbb{I} + s_i Z_i\Big), \quad (\text{ so that } \langle X_i\rangle = 0, \langle Z_i\rangle = s_i).$$

In this algorithm, we crucially use Grothendieck's identity (see for example Lemma 3.6.5, page 82 [41]), which is described in the following:

▶ **Lemma 9** (Grothendieck's Identity). *Let u_i, u_j be arbitrary unit vectors, $g \sim N(0, \mathbb{I})$ be a random vector, and s_i, s_j be their random signs obtained by the hyperplane rounding according to $s_i = \mathrm{sign}(\langle g, u_i\rangle)$. Then*

$$\mathbb{E}[s_i s_j] = K(\langle u_i, u_j\rangle), \text{ where } K(t) = \frac{2}{\pi}\arcsin(t).$$

The following is also a standard inequality used in the analysis of the Goemans-Williamson MaxCut approximation algorithm [18]:

▶ **Definition 10.** *For $t \in [0, 1]$ let*

$$R_A(t) = \frac{1 + K(t)}{1 + t}, \qquad \alpha_{\mathrm{GW}} = \min_{t\in[0,1]} R_A(t) \approx 0.878567.$$

Now we analyze the value of each term for the solution produced by Algorithm A compared to its value in the SDP solution. We start with the field terms in Lemma 11 followed by the Ising terms in Lemma 12.

▶ **Lemma 11.** *For each vertex i we have that $\mathrm{Tr}[\Pi_i^X \rho] = \frac{1}{2}$. Hence we have*

$$\sum_{i\in V} h_i \,\mathrm{Tr}[\Pi_i^X \rho] = \frac{1}{2}\sum_{i\in V} h_i \geq \frac{1}{2}\sum_{i\in V} h_i \frac{1 + x_i}{2} = \frac{\mathrm{SDP}_X}{2},$$

i.e. the total field contribution is at least $\frac{1}{2}\cdot \mathrm{SDP}_X$.

Proof. By construction $\mathrm{Tr}[\rho X_i] = 0$, so $\mathrm{Tr}[\Pi_i^X \rho] = (1+0)/2 = 1/2 \geq (1+x_i)/4$. ◀

▶ **Lemma 12.** *Let $t_{ij} = -J_{ij}\langle u_i, u_j\rangle$. Then for each edge $\{i,j\} \in E$,*

$$\mathbb{E}\big[w_{ij}\,\mathrm{Tr}[\Pi_{ij}^Z \rho]\big] = w_{ij}\frac{1+K(t_{ij})}{2} \geq w_{ij}\cdot\alpha_{\mathrm{GW}}\cdot\frac{1+t_{ij}}{2} = \alpha_{\mathrm{GW}}\cdot\mathrm{SDP}_E[i,j].$$

Hence the total Ising contribution is at least $\alpha_{\mathrm{GW}}\cdot\mathrm{SDP}_E$.

Proof. Since ρ is a product state with $\langle Z_i\rangle = s_i$, we have $\langle Z_iZ_j\rangle = s_is_j$ and

$$\mathrm{Tr}[\Pi_{ij}^Z\rho] = \frac{1-J_{ij}\langle Z_iZ_j\rangle}{2} = \frac{1-J_{ij}s_is_j}{2}.$$

Taking expectation and then applying Grothendieck's Identity (Lemma 9), we have that $\mathbb{E}[-J_{ij}s_is_j] = -J_{ij}K(\langle u_i,u_j\rangle) = K(-J_{ij}\langle u_i,u_j\rangle) = K(t_{ij})$, since K is odd. This gives $\mathbb{E}[\mathrm{Tr}[\Pi_{ij}^Z\rho]] = (1+K(t_{ij}))/2$. The inequality with α_{GW} holds by definition of α_{GW} on $t \in [0,1]$. For $t \leq 0$ the ratio is at least 1. ◀

Combining the two previous lemmata gives the following guarantee for Algorithm A:

▶ **Theorem 13.** *The product state $\rho^{(A)}$ output by Algorithm A satisfies*

$$\mathbb{E}[\mathrm{Tr}(H_{\mathrm{TFIM}'}\rho^{(A)})] \geq \alpha_{\mathrm{GW}}\cdot\mathrm{SDP}_E + \frac{1}{2}\cdot\mathrm{SDP}_X.$$

Where SDP_E and SDP_X denote the edge and field parts of the SOC-SDP objective.

4.2 A mixed X, ZZ algorithm

Algorithm B matches the SDP field marginals exactly and uses the remaining "budget" according to Lemma 4 to round the ZZ-marginals for edges. Thus, it achieves approximation factor 1 on the fields, and in the following (Lemma 19) we will bound the approximation guarantee on the Ising terms.

Algorithm B X, ZZ mixed solution.

Input: SOC-SDP solution (x_i, u_i) from Definition 7

1. For each vertex i, set $\alpha_i = \sqrt{1-x_i^2}$.
2. Sample $g \sim N(0, \mathbb{I})$.
3. Set $s_i = \mathrm{sign}(\langle g, u_i\rangle)$.
4. Output the product state $\rho = \bigotimes_{i\in V}\rho_i$ where

$$\rho_i = \frac{1}{2}\Big(\mathbb{I} + x_iX_i + \alpha_is_iZ_i\Big), \quad \text{so that } \langle X_i\rangle = x_i, \langle Z_i\rangle = s_i\alpha_i).$$

▶ Remark 14. Note that each ρ_i is a valid pure qubit state because its Bloch vector has length $x_i^2 + \alpha_i^2 = 1$.

▶ **Lemma 15.** *For each vertex i, Algorithm B satisfies*

$$\mathrm{Tr}[h_i\Pi_i^X\rho] = \frac{1+x_i}{2} = \mathrm{SDP}_X[i].$$

Hence the total field contribution equals the SOC-SDP field contribution SDP_X.

Proof. $\Pi_i^X = (\mathbb{I} + X_i)/2$ acts only on qubit i and ρ is a product state, so

$$\mathrm{Tr}[h_i \Pi_i^X \rho] = h_i \,\mathrm{Tr}[\Pi_i^X \rho_i] = h_i \frac{1 + \mathrm{Tr}[\rho_i X_i]}{2} = h_i \frac{1 + x_i}{2} = \mathrm{SDP}_X[i]. \qquad \blacktriangleleft$$

▶ **Lemma 16.** *Let $t_{ij} = -J_{ij} \langle u_i, u_j \rangle$, $\alpha_i = \sqrt{1 - x_i^2}$ as in Algorithm B. Then $\forall \{i, j\} \in E$,*

$$\mathbb{E}\big[\,\mathrm{Tr}[\Pi_{ij}^Z \rho]\big] = \frac{1 + \alpha_i \alpha_j K(t_{ij})}{2}.$$

Proof. Because $\rho = \bigotimes_k \rho_k$ is a product state, we have that $\langle Z_i Z_j \rangle_\rho = \mathrm{Tr}[\rho_i Z_i] \,\mathrm{Tr}[\rho_j Z_j] = (\alpha_i s_i)(\alpha_j s_j)$. Therefore

$$\mathrm{Tr}[\Pi_{ij}^Z \rho] = \frac{1 - J_{ij} \alpha_i \alpha_j s_i s_j}{2}.$$

Taking expectation and applying Grothendieck's Identity (Lemma 9) as in Lemma 12 gives $\mathbb{E}[-J_{ij} s_i s_j] = K(t_{ij})$ and hence the desired bound. $\blacktriangleleft$

We also need the following Lemma that relates the SDP Ising values t_{ij} with the "leftover" rounded values $\alpha_i \alpha_j$.

▶ **Lemma 17.** *If $t_{ij} \geq 0$ then $\alpha_i \alpha_j \geq t_{ij}^2$.*

Proof. The SOC anticommutation constraint (7) gives us $x_i^2 + c_{ij}^2 \leq 1$ from which we see that $\alpha_i = \sqrt{1 - x_i^2} \geq |c_{ij}|$, and similarly $\alpha_j \geq |c_{ij}|$. Thus $\alpha_i \alpha_j \geq c_{ij}^2 = t_{ij}^2$. $\blacktriangleleft$

▶ **Definition 18.** *For $t \in [0, 1]$ let*

$$R_B(t) = \frac{1 + t^2 K(t)}{1 + t}, \qquad \beta = \min_{t \in [0,1]} R_B(t).$$

Basic calculus (setting the derivative to zero) shows that $\beta \approx 0.716775$ achieved at $t \approx 0.58$.

Finally, we analyze the contribution of the Ising terms as compared to the SDP solution.

▶ **Lemma 19.** *For each edge $\{i, j\}$, Algorithm B satisfies*

$$\mathbb{E}\big[\,\mathrm{Tr}[\Pi_{ij}^Z \rho]\big] \geq \beta \cdot \frac{1 + t_{ij}}{2} = \beta \cdot \mathrm{SDP}_E[i, j].$$

Hence the total Ising contribution is at least $\beta \cdot \mathrm{SDP}_E$.

Proof. For $t_{ij} \in [0, 1]$, Lemmas 16 and 17 give

$$\mathbb{E}[\mathrm{Tr}[\Pi_{ij}^Z \rho]] = \frac{1 + \alpha_i \alpha_j K(t_{ij})}{2} \geq \frac{1 + t_{ij}^2 K(t_{ij})}{2} = R_B(t_{ij}) \cdot \frac{1 + t_{ij}}{2} \geq \beta \cdot \frac{1 + t_{ij}}{2}.$$

For $t_{ij} \leq 0$, note that $K(t_{ij}) \leq 0$ and $\alpha_i \alpha_j \leq 1$, hence $1 + \alpha_i \alpha_j K(t_{ij}) \geq 1 + K(t_{ij})$. Moreover, for $t \in [-1, 0]$ we have $K(t) \geq t$, so $1 + K(t_{ij}) \geq 1 + t_{ij}$, i.e. the ratio is at least 1. $\blacktriangleleft$

Combining Lemmata 15 and 19 gives the following approximation guarantee:

▶ **Theorem 20.** *The product state $\rho^{(B)}$ output by Algorithm B satisfies*

$$\mathbb{E}[\mathrm{Tr}(H_{\mathrm{TFIM}'} \rho^{(B)})] \geq \beta \cdot \mathrm{SDP}_E + 1 \cdot \mathrm{SDP}_X.$$

4.3 Combining Algorithms A & B

Proof idea. Algorithm A is strong on edges (factor α_{GW}) but weak on fields (trivial factor of only $1/2$) while Algorithm B is perfect on fields (factor 1) but weaker on edges (factor β). By defining p to be the fraction of the SDP coming from edges allows us to express each candidate's guarantee into an affine function of p. Taking the better candidate yields the maximum of these affine functions and the worst-case over instances is the minimum of that maximum over $p \in [0,1]$.

▶ **Theorem 21** (Two-candidate product rounding). *Let α_{GW} and β be as defined in Definitions 10 and 18 respectively. The algorithm which on an input TFIM instance executes Algorithms A and B and returns whichever of the two candidate outputs has higher energy achieves approximation ratio*

$$\gamma = \frac{1}{2} + \frac{1}{2} \cdot \frac{\alpha_{\mathrm{GW}} - 1/2}{\alpha_{\mathrm{GW}} + 1/2 - \beta} \approx 0.786$$

Proof. Recall that we have $\mathrm{SDP} = \mathrm{SDP}_E + \mathrm{SDP}_X$. Let

$$p = \frac{\mathrm{SDP}_E}{\mathrm{SDP}} \in [0,1], \text{ and correspondingly } 1-p = \frac{\mathrm{SDP}_X}{\mathrm{SDP}}.$$

Candidate A. From Theorem 13 we have

$$\mathbb{E}[\mathrm{Tr}(H_{\mathrm{CSP}}\rho^{(A)})] \geq \alpha_{\mathrm{GW}} \cdot \mathrm{SDP}_E + \frac{1}{2} \cdot \mathrm{SDP}_X \Rightarrow \frac{\mathbb{E}[\mathrm{Tr}(H_{\mathrm{CSP}}\rho^{(A)})]}{\mathrm{SDP}} \geq \frac{1}{2} + \left(\alpha_{\mathrm{GW}} - \frac{1}{2}\right) \cdot p.$$

Candidate B. From Theorem 20 we have

$$\mathbb{E}[\mathrm{Tr}(H_{\mathrm{CSP}}\rho^{(B)})] \geq \beta \cdot \mathrm{SDP}_E + 1 \cdot \mathrm{SDP}_X \Rightarrow \frac{\mathbb{E}[\mathrm{Tr}(H_{\mathrm{CSP}}\rho^{(B)})]}{\mathrm{SDP}} \geq 1 - (1-\beta) \cdot p.$$

Finally, we take the best of the two solutions and calculate the worst-case guarantee.

$$\frac{\mathbb{E}[\mathrm{Tr}(H_{\mathrm{CSP}}\rho)]}{\mathrm{SDP}} \geq \max\left\{\frac{1}{2} + \left(\alpha_{\mathrm{GW}} - \frac{1}{2}\right) \cdot p, 1 - (1-\beta) \cdot p\right\}.$$

Note that the two terms inside the maximum are respectively increasing and decreasing functions of p. They intersect at $p^\star = \frac{1/2}{\alpha_{\mathrm{GW}}+1/2-\beta}$, giving an overall worst-case approximation factor of $\gamma = 1 - (1-\beta)p^* \approx 0.786016$. ◀

5 An improved 0.82197 factor based on non-uniform interpolation

For the algorithm in the previous section we considered the two options of either setting each qubit to the purely Z direction in the Bloch sphere with signs chosen by rounding the SDP, or on the other hand taking the x_i values from the SDP and then using the remaining slack for the Z direction as before. In this section we interpolate between these two cases, by first scaling the x_i values by a *non-uniform* parameter $q_i \in [0,1], i \in V$ and then using the remaining slack for the Z direction.

The key point is that vertices with small SDP field marginals x_i should not necessarily receive any X-polarization in the rounded state because doing so may waste too much of the available Z-slack. We therefore apply a thresholding map to each x_i separately. For a parameter $c \in [1/2, 1]$, we would like to guarantee a factor c on the rounded X-marginals i.e., $\frac{1+\tilde{x}_i}{2} \geq c \cdot \frac{1+x_i}{2}$ so $\tilde{x}_1 \geq c(1+x_i) - 1$, so we define

$$f_c(x) = \max\{0,\, c(1+x) - 1\}, \qquad x \in [0,1].$$

From now on since $h_i \geq 0$ for all i and the SOC constraints depend on x_i only through x_i^2, we assume w.l.o.g. that in an optimal SDP solution $x_i \in [0,1]$ for each i. Since $c \leq 1$, the upper truncation at 1 never happens on $[0,1]$ except at the degenerate point $(c,x) = (1,1)$. Observe that $f_{1/2}(x) = 0$ for all $x \in [0,1]$, and $f_1(x) = x$ i.e., this family interpolates between Algorithm A and Algorithm B, but in a non-linear way.

Algorithm C Interpolated X, ZZ combined solution.

Input: SOC-SDP solution (x_i, u_i) from Definition 7, parameter $c \in [1/2, 1]$.

1. For each vertex i, $\tilde{x}_i = \max\{0, c(1+x_i) - 1\}$, $\alpha_i = \sqrt{1 - \tilde{x}_i^2}$.
2. Sample $g \sim N(0, \mathbb{I})$.
3. Set $s_i = \text{sign}(\langle g, u_i \rangle)$.
4. Output the product state $\rho(c) = \bigotimes_{i \in V} \rho_i$ where

$$\rho_i = \frac{1}{2}\Big(\mathbb{I} + \tilde{x}_i X_i + \alpha_i s_i Z_i\Big), \quad (\text{so that } \langle X_i \rangle = \tilde{x}_i = f_c x_i, \langle Z_i \rangle = s_i \alpha_i, s_i \in \{-1, +1\}).$$

Since $\tilde{x}_i^2 + \alpha_i^2 = 1$, each ρ_i is a valid pure single-qubit state.

We now analyze separately the field contribution and the Ising contribution. We begin with the field terms where map f_c guarantees a factor-c lower bound on every field term.

▶ **Lemma 22.** *For each field term (vertex) $i \in V$ we have that*

$$\text{Tr}[h_i \Pi_i^X \rho] = h_i \frac{1 + \langle X_i \rangle_\rho}{2} = h_i \frac{1 + f_c(x_i)}{2} \geq c \cdot \text{SDP}_X[i].$$

Hence the total field contribution of Algorithm C is at least $c \cdot \text{SDP}_X$.

Proof. The inequalities are immediate since by construction $\langle X_i \rangle_\rho = \tilde{x}_i$. It is therefore sufficient to show that $1 + f_c(x) \geq c(1+x)$ for all $x \in [0,1]$.
But $1 + f_c(x) = 1 + \max\{0, c(1+x) - 1\} = \max\{1, c(1+x)\} \geq c(1+x)$ and by multiplying with $h_i/2$ proves the claim. ◀

Now we proceed with the contribution of the Ising terms (edges) to the solution energy. As before, for an edge $\{i,j\} \in E$ we define $t_{ij} = -J_{ij}\langle u_i, u_j \rangle \in [-1,1]$. We first isolate the worst-case lower bound on the remaining Z budget.

▶ **Lemma 23.** *Fix an edge $\{i,j\} \in E$ and let $t = t_{ij}$. Then*

$$\alpha_i \alpha_j \geq 1 - f_c\left(\sqrt{1-t^2}\right)^2.$$

Proof. Since f_c is non-decreasing on $[0,1]$, the function $\sqrt{1 - f_c(x)^2}$ is non-increasing on $x \in [0,1]$. By the SOC-SDP constraints we have that $x_i^2 + t^2 \leq 1$ and $x_j^2 + t^2 \leq 1$. Since in an optimal SDP solution we can assume $x_i, x_j \geq 0$, we get $x_i \leq \sqrt{1-t^2}$ and $x_j \leq \sqrt{1-t^2}$. This gives

$$\alpha_i = \sqrt{1 - f_c(x_i)^2} \geq \sqrt{1 - f_c(\sqrt{1-t^2})^2},$$

and analogously for α_j. Multiplying the two inequalities we get the claim. ◀

We now define the edge ratio function that will give us the approximability guarantee.

▶ **Definition 24.** *For $c \in [1/2, 1]$ and $t \in [0, 1]$, define*

$$R_c(t) = \frac{1 + \left(1 - f_c(\sqrt{1-t^2})^2\right) K(t)}{1+t},$$

where $K(t) = \frac{2}{\pi} \arcsin(t)$, and define $\beta(c) = \min_{t \in [0,1]} R_c(t)$.

▶ **Lemma 25.** *For every Ising term (edge $\{i, j\} \in E$) we have that,*

$$\mathbb{E}\left[w_{ij} \operatorname{Tr}[\Pi_{ij}^Z \rho]\right] \geq \beta(c) \cdot \mathrm{SDP}_E[i, j].$$

Hence the total Ising contribution of Algorithm C is at least $\beta(c) \cdot \mathrm{SDP}_E$.

Proof. We proceed as in Lemma 19, but with the new values of α_i. Fix an edge $\{i, j\}$. Since ρ is a product state we have that $\langle Z_i Z_j \rangle_\rho = \langle Z_i \rangle_\rho \langle Z_j \rangle_\rho = (\alpha_i s_i)(\alpha_j s_j)$. Therefore

$$\operatorname{Tr}[\Pi_{ij}^Z \rho] = \frac{1 - J_{ij} \langle Z_i Z_j \rangle_\rho}{2} = \frac{1 + \alpha_i \alpha_j (-J_{ij} s_i s_j)}{2}.$$

As before, taking expectation and using Grothendieck's Identity, we have that

$$\mathbb{E}\left[-J_{ij} s_i s_j\right] = K(t_{ij}) \text{ where } t_{ij} = -J_{ij} \langle u_i, u_j \rangle \Longrightarrow \mathbb{E}\left[\operatorname{Tr}[\Pi_{ij}^Z \rho]\right] = \frac{1 + \alpha_i \alpha_j K(t_{ij})}{2}.$$

Case 1: $t_{ij} \in [0, 1]$. Then $K(t_{ij}) \geq 0$, so by Lemma 23,

$$\mathbb{E}\left[\operatorname{Tr}[\Pi_{ij}^Z \rho]\right] \geq \frac{1 + \left(1 - f_c(\sqrt{1 - t_{ij}^2})^2\right) K(t_{ij})}{2} = R_c(t_{ij}) \cdot \frac{1 + t_{ij}}{2} \geq \beta(c) \cdot \frac{1 + t_{ij}}{2}.$$

Case 2: $t_{ij} \in [-1, 0]$. Then, as before, $K(t_{ij}) \leq 0$, and since $\alpha_i \alpha_j \leq 1$, we have

$$1 + \alpha_i \alpha_j K(t_{ij}) \geq 1 + K(t_{ij}) \geq 1 + t_{ij} \quad \Longrightarrow \quad \mathbb{E}[\operatorname{Tr}[\Pi_{ij}^Z \rho]] \geq \frac{1 + K(t_{ij})}{2}.$$

We have that $K(t) \geq t$ for all $t \in [-1, 0]$, so $\mathbb{E}[\operatorname{Tr}[\Pi_{ij}^Z \rho]] \geq \frac{1 + t_{ij}}{2}$. But $(1 + t_{ij})/2$ is exactly the SDP value (divided by w_{ij}). Thus the approximation ratio on such an edge is at least $\mathbb{E}[\operatorname{Tr}[\Pi_{ij}^Z \rho]] / ((1 + t_{ij})/2) \geq 1$.

Combining the two cases gives

$$\mathbb{E}[\operatorname{Tr}[\Pi_{ij}^Z \rho]] \geq \beta(c) \cdot \frac{1 + t_{ij}}{2} = \beta(c) \cdot \frac{\mathrm{SDP}_E[i, j]}{w_{ij}}.$$

Multiplying by w_{ij} proves the claim. ◀

We can now combine the field and edge bounds.

▶ **Theorem 26.** *For every $c \in [1/2, 1]$, Algorithm C outputs a product state ρ satisfying*

$$\mathbb{E}[\operatorname{Tr}(H'_{\mathrm{TFIM}} \rho)] \geq \beta(c) \cdot \mathrm{SDP}_E + c \cdot \mathrm{SDP}_X \geq \min\{\beta(c), c\} \cdot \mathrm{SDP}.$$

Consequently, Algorithm C is a $\min\{\beta(c), c\}$-approximation algorithm for TFIM.

Proof. The first inequality is exactly the combination of Lemma 22 and Lemma 25. The second inequality follows because

$$\beta(c) \cdot \mathrm{SDP}_E + c \cdot \mathrm{SDP}_X \geq \min\left\{\beta(c), c\right\}\left(\mathrm{SDP}_E + \mathrm{SDP}_X\right) = \min\left\{\beta(c), c\right\} \cdot \mathrm{SDP}.$$

Finally, since SDP $\geq$ OPT by Lemma 8, the same factor holds with respect to the true optimum. ◀

To optimize the guarantee, we choose c so that the two lower bounds c and $\beta(c)$ are balanced. We can easily see that the function $\beta(c)$ is decreasing in c on $[1/2, 1]$. The equation $\beta(c) = c$ has a solution $c^\star \approx 0.8219712361$. At this value we get $t^\star \approx 0.58154$.

▶ **Corollary 27.** *Taking $c = 0.82197$ in Algorithm C yields a 0.8219-approximation algorithm for TFIM.*

Proof. By Theorem 26, it suffices to verify that $\beta(0.82197) \geq 0.82197$. This is a one-dimensional inequality in the variable $t \in [0, 1]$:

$$R_{0.82197}(t) = \frac{1 + \left(1 - f_{0.8219}(\sqrt{1-t^2})^2\right) \frac{2}{\pi} \arcsin(t)}{1+t} \geq 0.8219 \qquad \text{for all } t \in [0,1].$$

Numerical Optimization gives $t \approx 0.58154$, where $R_{0.82197}(t) \approx 0.821972 > 0.82190$. Thus $\beta(0.82197) \geq 0.82197$, proving the claim. ◀

▶ Remark 28. A uniform interpolation where for each vertex i, set $\alpha_i(q) = \sqrt{1-(qx_i)^2}$ using the same parameter q, yields 0.8156-approximation guarantee.

6 A product-state 169/180 optimality gap on a triangle instance

We give a concrete 3-qubit purely antiferromagnetic TFIM instance where product states provably cannot achieve the true optimum. This gives an upper bound for any method that is restricted to output product states. Let $V = \{0, 1, 2\}$ and $E = \{\{0, 1\}, \{1, 2\}, \{0, 2\}\}$ with $w_{ij} = 1$ and $h_i = g$ with $g = \frac{3}{5}$. Take $J_{01} = J_{12} = J_{02} = +1$.

Let H_t denote the corresponding Hamiltonian on this instance. This is a 3 qubit Hamiltonian and as such a $2^3 \times 2^3$ Hermitian matrix. A direct diagonalization gives the spectrum

$$\left\{ \frac{18}{5}, \ \frac{16}{5} \ (\times 2), \ \frac{13}{5} \ (\times 2), \ \frac{8 \pm \sqrt{19}}{5}, \ \frac{4}{5} \right\},$$

so the maximum eigenvalue is $\frac{18}{5}$. The interesting direction is to upper bound the value achievable by any product state.

▶ **Lemma 29.** *Let $\mathrm{OPT}_{\mathrm{prod}} = \max_{\rho \text{ product}} \mathrm{Tr}[H_t \rho]$. For this instance $\mathrm{OPT}_{\mathrm{prod}} = 169/50$.*

Proof. We have $\mathrm{OPT}_{\mathrm{prod}} = \max_{\rho = \rho_1 \otimes \rho_2 \otimes \rho_3} \mathrm{Tr}[H_t \rho]$. We will represent each ρ_i by its Bloch vector (x_i, y_i, z_i). Note that trivially the optimum is reached at a pure state so we have $x_i^2 + y_i^2 + z_i^2 = 1$. Further, we may assume that $x_i \geq 0$ and $y_i = 0$, since otherwise replacing (x_i, y_i, z_i) with $(\sqrt{x_i^2 + y_i^2}, 0, z_i)$ improves the solution. Hence $x_i = \sqrt{1 - z_i^2}$.

Now we will write the objective as a function of (z_0, z_1, z_2). Since $\langle Z_i Z_j \rangle = z_i z_j$ and $\langle X_i \rangle = x_i$ we have

$$\mathrm{Tr}[H_t \rho] = \sum_{\{i,j\} \in E} \frac{1 - J_{ij} z_i z_j}{2} + \frac{g}{2} \sum_{i=0}^{2} (1 + x_i).$$

Putting $J_{ij} = +1$ for all edges, $g = 3/5$ and $x_i = \sqrt{1 - z_i^2}$ we obtain

$$F(z) = \frac{1}{2}(1 - z_0 z_1) + \frac{1}{2}(1 - z_1 z_2) + \frac{1}{2}(1 - z_0 z_2) + \frac{3}{10} \sum_{i=0}^{2} (1 + \sqrt{1 - z_i^2}),$$

and so our optimization problem is transformed to a simple optimization problem in the cube $[-1, 1]^3$: $\mathrm{OPT}_{\mathrm{prod}} = \max_{|z_i| \leq 1} F(z_0, z_1, z_2)$.

Since $g > 0$, an optimal solution cannot have $|z_i| = 1$ (equivalently $x_i = 0$) since otherwise perturbing that qubit slightly so that z_i decreases by ϵ and x_i increases by $\sqrt{\epsilon}$ changes the edge terms only by $\approx \epsilon^2$ but increases the field contribution by ϵ.

Now we can differentiate F with respect to each z_i. The first-order stationary conditions gives us the system

$$x_0(z_1 + z_2) = -gz_0, \qquad x_1(z_0 + z_2) = -gz_1, \qquad x_2(z_0 + z_1) = -gz_2, \qquad (g = 3/5).$$

Solving this system over $|z_i| < 1$ gives the following critical points (i) $z_0 = z_1 = z_2 = 0$ (hence $x_0 = x_1 = x_2 = 1$); (ii) up to relabeling, one coordinate is 0 and the other two are opposite:

$$z_a = 0, \qquad z_b = -z_c = \pm 4/5, \qquad x_a = 1, \qquad x_b = x_c = 3/5.$$

Now we evaluate F on these candidate solutions. At $(z_0, z_1, z_2) = (0, 0, 0)$ we have $x_i = 1$ and thus $F = \frac{3}{2} + \frac{3}{10} \cdot 3 \cdot 2 = \frac{33}{10} = 3.3$. At (ii), say $(z_0, z_1, z_2) = (0, 4/5, -4/5)$ with $(x_0, x_1, x_2) = (1, 3/5, 3/5)$, we get

$$\text{edges} = \frac{1}{2}(1-0)+\frac{1}{2}\left(1-\left(-\frac{16}{25}\right)\right)+\frac{1}{2}(1-0) = \frac{91}{50}, \quad \text{fields} = \frac{3}{10}\left[(1+1)+\left(1+\frac{3}{5}\right)+\left(1+\frac{3}{5}\right)\right] = \frac{78}{50}.$$

So $F = 91/50 + 78/50 = 169/50$.

It remains to handle the case where all $z_i \neq 0$. This can also be done analytically: we can see that all such points must have mixed signs and the stationary equations force every such critical point, up to permutation and global sign, to have the form $(a, -b, -b)$, $a, b > 0$, thus we can reduce the computations to only one variable $r = \sqrt{1 - b^2}$. From this, with direct computations, we derive a cubic equation for r, which gives us that $r < 13/15$, and rewriting the objective in terms of r shows that its objective value is always strictly smaller than $169/50$. ◀

▶ **Corollary 30.** *For this instance,*

$$\frac{\mathrm{OPT}_{\mathrm{prod}}}{\mathrm{OPT}} = \frac{169/50}{18/5} = \frac{169}{180} \approx 0.938888.$$

Consequently, no algorithm restricted to output product states can guarantee a worst-case approximation ratio exceeding $169/180$ *for arbitrary TFIM instances.*

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