

Lower bounds to variational problems with guarantees

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Variational methods play an important role in the study of quantum many-body problems, both in the flavor of classical variational principles based on tensor networks as well as of quantum variational principles in near-term quantum computing. This work stresses that for translationally invariant lattice Hamiltonians with periodic boundary conditions, one can easily derive efficiently computable lower bounds to ground state energies that can and should be compared with variational principles providing upper bounds. As small technical results, it is shown that (i) the Anderson bound and a (ii) common hierarchy of semidefinite relaxations both provide approximations with performance guarantees that scale as a constant in the energy density for cubic lattices. (iii) Also, the Anderson bound is systematically improved as a hierarchy of semidefinite relaxations inspired by the quantum marginal problem.

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I. INTRODUCTION

Variational principles are for good reason ubiquitous in the study of quantum many-body systems. They allow for achieving insights into the physics of quantum many-body systems in ways that are hard to obtain by any other method, in particular in situations when strong correlations are dominant or when an instance of the sign problem occurs so that other workhorses of the numerical study of quantum many-body systems such as density functional theory [1] or quantum Monte Carlo methods [2] are being challenged in their performance. A ground state of a local many-body Hamiltonian H_N defined on a lattice $\mathcal{L}$ composed of N sites or vertices each of which is associated with a d -dimensional quantum system is even defined as a state satisfying

$$\rho_G := \operatorname{argmin}_{\rho \in \mathcal{S}[(\mathbb{C}^d)^{\otimes N}]} \operatorname{tr}(\rho H_N). \quad (1)$$

This is the solution of a variational principle over all quantum states ρ defined on these N degrees of freedom. A substantial body of literature on the study of strongly correlated quantum systems with many degrees of freedom is hence dedicated to formulating meaningful tractable *ansatz* classes to tackle this general variational principle. Naturally, if one merely optimizes over certain families of quantum states $\rho \in \mathcal{T}[(\mathbb{C}^d)^{\otimes N}]$, the latter being a suitable subset of all quantum states, one arrives at quantum states providing an upper bound to the ground state energy density

$$e_{\min}(H_N) := \frac{1}{N} \min_{\rho \in \mathcal{S}[(\mathbb{C}^d)^{\otimes N}]} \operatorname{tr}(\rho H_N) = \frac{1}{N} \lambda_{\min}(H_N). \quad (2)$$

This idea has presumably become most prominent in the study of tensor network states [3–5] where classically efficient (in

memory storage, but also in computational complexity at least in approximation) *ansatz* classes are being used to generate excellent approximations of true ground states. The basis of their functioning is that common ground states of local Hamiltonians are much less entangled than they could be [6], allowing for efficient approximations. Indeed, ground states of gapped one-dimensional local Hamiltonians can basically be parametrized by the solutions of such variational principles, in fact by instances of matrix product states.

An alternative *ansatz* that is increasingly becoming popular is that of using quantum circuits in what is called the variational quantum eigensolver [7,8]: In this context, one thinks of near-term quantum computers that have the ability to prepare states from a parametrized family of quantum states, for which the expectation value of the given Hamiltonian is then estimated and computed from measurement data. A limitation of such *ansätze* is the often relatively low expressivity of the parametrized family of states; at the same time, in contrast to classical approaches they do not require an efficient classical contraction. What is more, the training of such variational quantum algorithms based on expectation values requires many samples [9], gradients can be small so that training is difficult [10,11], and in instances, they can also be “dequantized” by proposing classical algorithms for the same task. That said, they remain an important application of near-term quantum computers [12,13]. Both *ansätze* deliver upper bounds to the energy density of the ground state.

Either way, as such, by construction such methods do not provide any certificate of the quality of the approximation of the ground state energy. This may be less of an issue for tensor network methods that reach enormous precision, but even there certificates are helpful. It surely applies to quantum variational approaches that are presently within reach. This article stresses that lower bounds of the ground state energy that provide precisely such certificates can be found, often with little programming effort [14–18]. A similar point has also been made for variational quantum eigensolvers in Ref. [19].

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For simplicity, throughout this work, we consider translationally invariant local Hamiltonians with nearest-neighbor interactions, defined on cubic lattices $\mathcal{L}$ of size $|\mathcal{L}| := N = n^D$, naturally equipped with periodic boundary conditions. This means that the Hamiltonian takes the form

$$H_N = \sum_{j \in \mathcal{L}} \tau_j(h), \quad (3)$$

where τ_j places the nearest-neighbor Hamiltonian term h at a root site $j \in \mathcal{L}$ of a lattice hosting a d -dimensional quantum degree of freedom. For conceptual simplicity, we assume h to be supported on 2^D sites.

In this work, it is shown that common such lower bounds can be seen to feature performance guarantees that scale as $O(1)$ in the system size N for the ground state energy density with a small constant that can be tightly bounded. Also, the Anderson bound is improved. The arguments presented here are all elementary, but on a conceptual level, it is still worth stressing that any variational eigensolver has to deliver a value that is more accurate than a constant in N in order to deliver a meaningful estimate for the ground state energy. In this sense, the results stated here can be seen as (immediate instances of) “dequantization” results, in that they place stringent demands on any quantum algorithm aimed at obtaining a quantum advantage when estimating ground state energies. For what follows, we define as the central quantity of this work

$$e_{\min} := \limsup_{n \rightarrow \infty} e_{\min}(H_{n^D}) \quad (4)$$

as the asymptotic ground state energy density.

II. A PERFORMANCE GUARANTEE FOR THE ANDERSON BOUND

The Anderson bound [14] is a remarkably simple lower bound to the ground state energy of quantum many-body Hamiltonians, basically merely exploiting the triangle inequality of the operator norm $\|\cdot\|$ applied to the Hamiltonian equipped with a negative sign see Fig. 1. It is conceptually easy and is implementable with a small programming effort, of less than 1 h for a one-dimensional Hamiltonian problem. The performance of the bound is depicted in Fig. 2 for the Heisenberg Hamiltonian in one spatial dimension. In this section, we see that it actually always delivers an approximation of the ground state energy density up to a small constant in N , in fact, arbitrarily small, with a computational effort that is exponential in m .

Proposition 1 (Performance guarantee of the Anderson bound). Consider a family of translationally invariant Hamiltonians of the form (3) on a cubic lattice in some spatial dimension D with periodic boundary conditions, indexed by the system size $N = n^D$, and let $\lambda_{\min}(h_m)$ be the smallest eigenvalue of a cubic patch h_m of H_N on m^D sites, with open boundary conditions, then

$$A(m, D) := \frac{\lambda_{\min}(h_m)}{(m-1)^D} \leq e_{\min}, \quad (5)$$

$$|e_{\min} - A(m, D)| \leq \frac{D}{m} \|h\| - \lambda_{\min}(h_m) \left[\frac{1}{(m-1)^D} - \frac{1}{m^D} \right]. \quad (6)$$

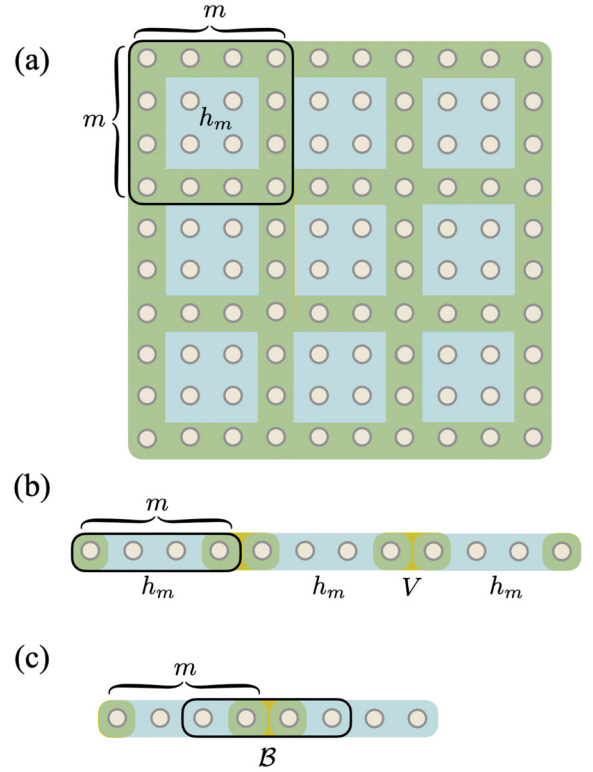


FIG. 1. (a) The configuration in the original Anderson bound applied to a two-dimensional translationally invariant lattice system. For the periodic boundary conditions, the last row and column are identified with the first one. (b) The configuration in one spatial dimension used to show the performance guarantee of the Anderson bound. (c) The configuration employed for the improved Anderson bound based on semidefinite programming and the marginal problem, again applied to one spatial dimension.

Proof. The first inequality, first stated in Ref. [14] and here adapted to the asymptotic limit of large cubic lattices, is an immediate consequence of the following basic and still profound insight: One composes a Hamiltonian of $N = [(m-1)J]^D$

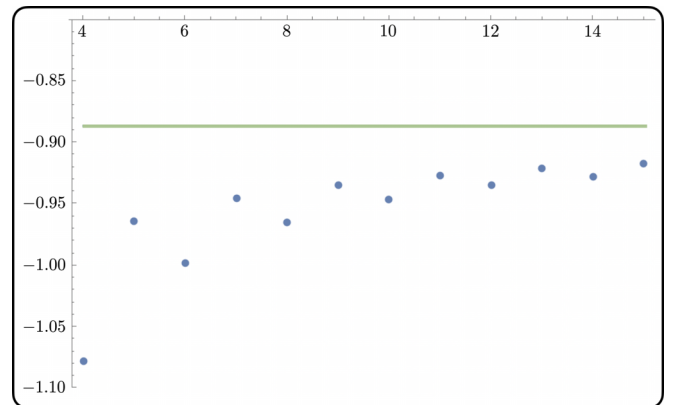


FIG. 2. The Anderson bound for the one-dimensional Heisenberg model $H = \frac{1}{2} \sum_j \tau_j(X \otimes X + Y \otimes Y + Z \otimes Z)$ as a function of the patch size m until $m = 15$, featuring a noteworthy even-odd effect. The straight line represents the exact ground state energy density, $e_{\min} = -2 \log(2) + 1/2$.

sites into J^D overlapping parts [see Fig. 1(a)]

$$H_N = \sum_{s \in I_{m,J}} \tau_s(h_m), \quad (7)$$

where $I_{m,J} := \{(m-1)(j_1-1)+1, \dots, (m-1)(j_D-1)+1\} : j_1, \dots, j_D = 1, \dots, J\} \subset \mathcal{L}$. Then, clearly,

$$\lambda_{\min}(H_N) \geq \sum_{s \in I_{m,J}} \lambda_{\min}(h_m) = J^D \lambda_{\min}(h_m), \quad (8)$$

where the first bound follows from the fact that the smallest eigenvalue of H_N is lower bounded by the sum of the smallest eigenvalues of each of the J^D parts consisting of m^D sites each. For $J \rightarrow \infty$, this gives the first statement of Eq. (5). The performance guarantee can be shown by considering a different partition [see Fig. 1(b)],

$$H_N = \sum_{s \in K_{m,J}} \tau_s(h_m) + V_N, \quad (9)$$

where $K_{m,J} := \{[m(j_1-1)+1, \dots, m(j_D-1)+1] : j_1, \dots, j_D = 1, \dots, J\} \subset \mathcal{L}$, and hence $n = Jm$, $N = n^D$, and where V_N is the remainder term that consists of nearest-neighbor terms connecting the slightly larger patches. Let us define $|\phi\rangle := \operatorname{argmin}_{|\psi\rangle} \langle \psi | h_m | \psi \rangle$. Then

$$\begin{aligned} \frac{\lambda_{\min}(H_N)}{N} - \frac{\lambda_{\min}(h_m)}{(m-1)^D} &= \min_{|\psi\rangle} \frac{\langle \psi | H_N | \psi \rangle}{N} - \frac{\langle \phi | h_m | \phi \rangle}{(m-1)^D} \\ &\leq \langle \phi | h_m | \phi \rangle \frac{J^D}{N} + \frac{1}{N} \|V_N\| - \langle \phi | h_m | \phi \rangle \frac{1}{(m-1)^D} \\ &\leq \langle \phi | h_m | \phi \rangle \frac{J^D}{N} + m^{D-1} \|h\| \frac{DJ^D}{N} - \langle \phi | h_m | \phi \rangle \frac{1}{(m-1)^D} \\ &= \lambda_{\min}(h_m) \left[\frac{1}{m^D} - \frac{1}{(m-1)^D} \right] + \frac{D}{m} \|h\|, \end{aligned} \quad (10)$$

where the first inequality follows from the fact that the minimum of $\min(\rho h_m)$ over quantum states ρ takes the smallest value for $\langle \phi | h_m | \phi \rangle$, the second from the triangle inequality of the operator norm. Then, one encounters fewer than Dm^{D-1} boundary terms in a cubic patch in D dimensions involving m^D many vertices (avoiding double counting); and again, the triangle inequality of the operator norm is used. As before, the statement follows for $J \rightarrow \infty$. ■

III. PERFORMANCE GUARANTEES FOR SEMIDEFINITE RELAXATIONS

Similar performance guarantees can be shown for common hierarchies of semidefinite relaxations [20] of finding the ground states of local Hamiltonians [15–18], giving rise to in practice commonly much tighter bounds than those provided by Anderson-type bounds [16]. The core idea of these approaches is very simple: The constraint of quantum states being positive semidefinite $\rho \geq 0$ is relaxed to operators ω satisfying $\operatorname{tr}(\omega O^\dagger O) \geq 0$ for suitable operators O . In a next step, the quantum state ω is eliminated. Since the constraint of quantum states being positive semidefinite is relaxed, one naturally arrives at lower bounds to ground state energies.

Concretely, for a distinguished lattice site j , consider a set $\mathcal{M}$ of cardinality $|\mathcal{M}| =: C$ of operators $O_a \in \mathcal{M}$ that has the property that the Hamiltonian term on this site can be written as

$$\tau_j(h) = \sum_{a,b} c_{a,b} O_a^\dagger O_b, \quad (11)$$

with $c_{a,b} \in \mathbb{C}$ for $a, b = 1, \dots, C$. The set of sites on which all operators in $\mathcal{M}$ are nontrivially supported is denoted as $\mathcal{S}$, which at the same time contains by construction the support of $\tau_j(h)$ (but which may be substantially larger). This set is being seen as the root set of operators that then acts in a translationally invariant fashion on each lattice site in the same fashion. The methods discussed in Refs. [15–18] essentially amount to identifying suitable such sets of operators. The operators considered in $\mathcal{M}$ will feature algebraic relations (such as commutation or anticommutation relations). We consider again translationally invariant settings, with

$$\mathcal{O}_N := \{\tau_j(O_a) : \forall j \in \mathcal{L}, a = 1, \dots, C\} \quad (12)$$

being defined as translates of the root set of operators $\mathcal{M}$, giving rise to a set of cardinality $|\mathcal{O}_N| =: D_N$. To express the lower bound, we define the matrix X with

$$X_{a,b} := \operatorname{tr}(O_a^\dagger O_b \omega) \quad (13)$$

for $a, b = 1, \dots, D_N$. The matrices $X \in \mathbb{C}^{D_N \times D_N}$ will again be taken to be translationally invariant, in that

$$X_{a,b} = \operatorname{tr}[\tau_j(O_a^\dagger) \tau_j(O_b) \omega] \quad (14)$$

for all $j \in \mathcal{L}$ and all $a, b = 1, \dots, D_N$. The above constraints between the operators will be reflected by expressions of the form $\operatorname{tr}(XR) = 1$ for suitable matrices $R \in \mathbb{C}^{D_N \times D_N}$. The constraints immediately also act in a translationally invariant fashion: We denote the set of matrices $R \in \mathbb{C}^{D_N \times D_N}$ that reflect both the local algebraic constraints as well as the translational invariance in Eq. (14) as $\mathcal{X}_N$. For all $X \in \mathbb{C}^{D_N \times D_N}$ that satisfy $X \geq 0$ and $\operatorname{tr}(XR) = 1$ for all $R \in \mathcal{X}_N$,

$$\sum_{a,b} \alpha_a^* \alpha_b \operatorname{tr}(O_a^\dagger O_b \rho) = \sum_{a,b} \alpha_a^* \alpha_b X_{a,b} \geq 0 \quad (15)$$

will hold true for all $\alpha \in \mathbb{C}^{D_N}$, allowing to devise a lower bound to the ground state energy density. In fact, these bounds will again be lower bounds with a guaranteed constant error.

Proposition 2 (Performance guarantee of semi-definite bounds). The solution x_N of the semidefinite problem

$$\text{minimize } \operatorname{tr}(hX), \quad (16)$$

$$\text{subject to } X \geq 0, \quad (17)$$

$$\operatorname{tr}(XR) = 1 \quad \forall R \in \mathcal{X}_N, \quad (18)$$

where $\mathcal{X}_N$ reflects algebraic constraints as well as translational invariance, satisfies $x_N \leq e_{\min}(H_N) \leq x_N + O(1)$.

Proof. Since (15) is true for all $\alpha \in \mathbb{C}^{D_N}$ exactly if $X \geq 0$, and since

$$\sum_{a,b} h_{a,b} \operatorname{tr}(O_a O_b \omega) = \sum_{a,b} h_{a,b} X_{a,b} = \operatorname{tr}(hX), \quad (19)$$

we get the above lower bounds as the solution of the convex optimization problem Eqs. (16)–(18), as the energy minimization problem is relaxed to a semidefinite problem. We will continue the argument by showing that these bounds will scale as a constant in the energy density. For this, we consider a set of fixed lattice sites $\mathcal{T}$ independent of N that is a superset of the set $\mathcal{S}$ that hosts $\tau_j(h)$ but which may be substantially larger than its support, $\mathcal{S} \subset \mathcal{T}$. The strategy will be to construct bounds that are even lower bounding the ones from Proposition 2, but that already give rise to a constant energy approximation from below. These lower bounds are given by the solution of semidefinite problems with (16) and (18), where (17) is relaxed to the principal submatrix associated with $\mathcal{T}$ satisfying

$$X|_{\mathcal{T}} \geq 0. \quad (20)$$

This will give rise to lower bounds of the original semidefinite optimization problem, as $X \geq 0$ implies that the principal submatrix $X|_{\mathcal{T}}$ of the matrix X is also positive semidefinite. Since no constraint in the problem involves the system size any longer, and the only constraints dependent on N in $\mathcal{X}_N$ enforce translational invariance, the solution of this new semidefinite problem

$$\text{minimize} \quad \text{tr}(hX), \quad (21)$$

$$\text{subject to} \quad X|_{\mathcal{T}} \geq 0, \quad (22)$$

$$\text{tr}(XR) = 1 \quad \forall R \in \mathcal{X}_N \quad (23)$$

scales as $O(1)$ in N . This implies that the solution of the original semidefinite problem in Proposition 2 satisfies $x_N \leq e_{\min}(H_N) \leq x_N + O(1)$. At the same time, it is clear that by enlarging the set $\mathcal{M}$, the actual ground state energy $e_{\min}(H_N)$ can be arbitrarily well approximated from below. ■

IV. A HIERARCHY OF IMPROVED ANDERSON BOUNDS

The Anderson bound as is provides strikingly good lower bounds of the energy density up to small constant errors at very little effort. For this reason, the question arises whether it can be systematically improved. Resorting to the quantum marginal problem, one can, in fact, improve the Anderson bound. For this, consider again a configuration similar to the one used in Proposition 1, described in Eq. (9), and in fact employ an Anderson bound for twice the patch size. This amounts to the solution to the convex optimization problem

$$\text{minimize} \quad \text{tr}(\omega h_{2m}) \quad (24)$$

$$\text{subject to} \quad \omega \geq 0, \quad \text{tr}(\omega) = 1 \quad (25)$$

over quantum states defined on $(\mathbb{C}^d)^{\otimes 2m}$. For any such bound, the computational effort is exponential in m , so while the ground state of h_m may be within reach, that of h_{2m} may not be. Inspired by the quantum marginal problem [21,22], this problem can, however, be relaxed in the following way, to a family of efficiently solvable semidefinite problems [see also Fig. 1(c), where the overlapping sites are referred to as $\mathcal{B}$] that strictly generalize the Anderson bound.

Proposition 3 (Improved Anderson bounds). For a one-dimensional translationally invariant Hamiltonian H_N and an

integer s with $s \leq m$, the convex relaxation of the optimization problem in Eqs. (24) and (25) can for $s = 1, \dots, m$ be relaxed to the semidefinite optimization problem

$$\text{minimize} \quad 2 \text{tr}(\omega h_m) + \text{tr}[(\mathbb{I} \otimes h \otimes \mathbb{I})\sigma], \quad (26)$$

$$\sigma|_{\{1, \dots, s\}} = \omega|_{\{m-s+1, \dots, m\}}, \quad (27)$$

$$\sigma|_{\{s+1, \dots, 2s\}} = \omega|_{\{1, \dots, s\}}, \quad (28)$$

$$\sigma \geq 0, \quad \omega \geq 0, \quad \text{tr}(\sigma) = \text{tr}(\omega) = 1, \quad (29)$$

the optimal value $x_{m,s}$ of which satisfies

$$\frac{x_{m,s}}{(2m-1)} \leq \frac{x_{m,m}}{(2m-1)} \leq e_{\min}. \quad (30)$$

Proof. This can be easily seen as a relaxation of the full problem for $s = m$: Then the minimization delivers exactly the smallest eigenvalue $\lambda_{\min}(h_{2m})$ of h_{2m} , so that

$$\frac{x_{m,m}}{(2m-1)} = \frac{\lambda_{\min}(h_{2m})}{(2m-1)} \leq e_{\min} \quad (31)$$

delivers precisely the Anderson bound for $2m$ sites. For smaller values $s = 1, \dots, m-1$, one merely requires ω and σ to be identical on a subset of sites, hence relaxing the problem, leading to smaller and less tight lower bounds,

$$\frac{x_{m,s}}{(2m-1)} \leq \frac{x_{m,t}}{(2m-1)} \leq \frac{x_{m,m}}{(2m-1)} \leq e_{\min} \quad (32)$$

for $t = s, \dots, m$. ■

Hence, making use of the quantum marginal problem, one arrives at a hierarchy of new bounds.

V. SUMMARY AND OUTLOOK

This work emphasizes that one can easily equip upper bounds to ground states obtained by resorting to classical or quantum variational principles with concomitant lower bounds: These bounds certify the quality of the variational *ansatz*. As technical results, performance guarantees of Anderson bounds and of semidefinite relaxations are proven. What is more, an improved Anderson bound is presented. The upshot is that certified bounds to the energy density up to small constant $O(1)$ in the system size—for the Anderson bound even quantitative ones—are easy to get classically.

All lower bounds are comparably simple. One may argue, however, that it is their simplicity that renders them useful: Again, they can be interpreted as “dequantization statements.” It is sometimes underappreciated that one can easily classically approximate ground state energy densities up to a small constant error from below: This places stringent demands on quantum simulations aimed at producing such approximations. Any quantum simulation aimed at approximating ground state energies hence has to deliver approximations that scale more favorably compared to this in order to possibly outperform classical computations. Reference [23] makes a similar point for systems of quantum chemistry, stressing that estimating the ground state energy of a local Hamiltonian when given, as an additional input, a state sufficiently close to the ground state, can be solved efficiently with constant precision on a classical computer. This work also provides a “proof

pocket,” providing a variational quantum eigensolver with rigorous performance guarantees [24], and hence contributes to making near-term quantum computing more reliable and quantitative.

The results stated are clearly not in contradiction with the famous quantum Probabilistically Checkable Proofs (PCP) conjecture [25]. After all, this conjecture states that it remains quantum Merlin-Arthur (QMA) hard to approximate the ground state energy even up to an error γn for some absolute constant $0 < \gamma < 1$, where n is the number of local terms in the Hamiltonian. Obviously, the above bounds produce exactly such an energy approximation, which only once again implies that the statement of the quantum PCP conjecture cannot be expected to be tight for cubic lattices. It is also worth noting that all the mentioned bounds apply equally well to fermionic Hamiltonians [26,27] which have again moved to the focus of attention recently, not the least as the precise scaling of the ground state energy of the Sachdev-Ye-Kitaev (SYK) model [28–30] of random degree polynomials has become interesting. It might also be fruitful to compare

the discussed bounds with improvements of Temple’s lower bound [31]. It is the hope that this work can contribute to the development of benchmarks for variational principles in both the classical and quantum reading.

Note added. Recently, I became aware of a related but different relaxation of the infinite translationally invariant ground state problem [32] compared to what is stated as Proposition 3. It would be interesting to compare the two relaxations, which is left to future work.

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