

Obstacles to Variational Quantum Optimization from Symmetry Protection Supplementary Material

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A QAOA state preparation circuit

In this section we construct a quantum circuit that prepares the level- p QAOA state for any Ising-type Hamiltonian

$$C = \sum_{(j,k) \in E} J_{j,k} Z_j Z_k$$

defined on a graph $G = (V, E)$ with n vertices and maximum vertex degree D . This includes the MaxCut Hamiltonian as a special case. Let

$$U = \prod_{a=1}^p e^{i\beta_a B} e^{i\gamma_a C}$$

be the requisite circuit. For simplicity, we ignore the initial layer of Hadamard gates that prepares the $|+\rangle^n$ state.

Lemma A.1. *The unitary U can be realized by a circuit of depth $d \leq p(D+2)$ composed of 1-qubit and 2-qubit gates. If the graph G is D -regular and bipartite then $d \leq p(D+1)$.*

Proof. By Vizing's theorem [24] there is an edge coloring of G with at most $D+1$ colors. Let $E = E_1 \cup \dots \cup E_{D+1}$ be such a coloring. For each color $c \in \{1, \dots, D+1\}$ define a unitary

$$V_c = \prod_{(j,k) \in E_c} e^{i\gamma J_{j,k} Z_j Z_k}$$

Note that V_c is a depth-1 circuit since all edges in E_c are disjoint. Then each entangling layer $e^{i\gamma_a C}$ can be realized by a depth $D+1$ circuit $V_1 V_2 \dots V_{D+1}$. Each layer $e^{i\beta_a B}$ is a product of single-qubit gates, which has depth one. Thus U has depth at most $p(D+2)$.

If G is D -regular and bipartite, we may reduce the number of edge colors from $D+1$ to D since all bipartite graphs are D -edge-colorable by König's line coloring theorem. We illustrate the construction of the circuit on Figure 1 for the case $D=3$ and $p=1$. \square

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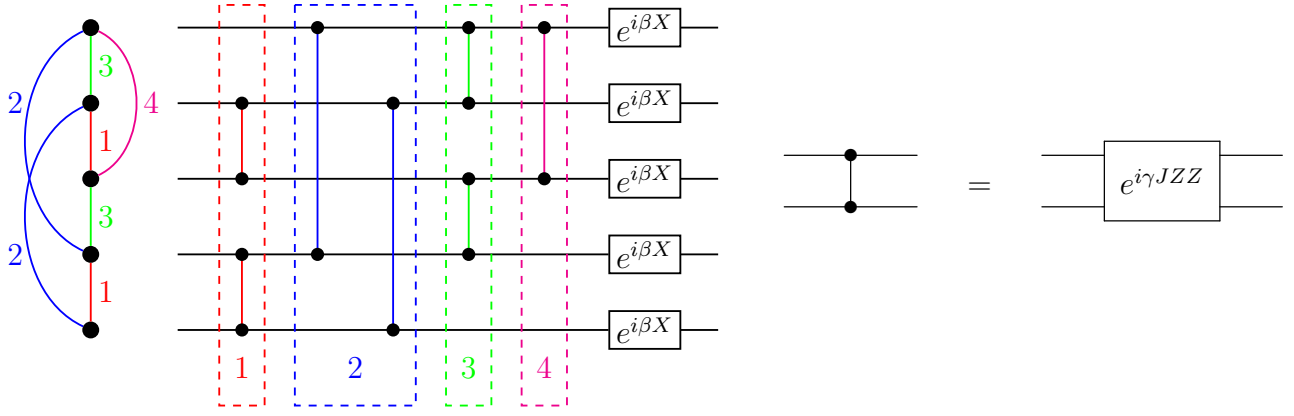


Figure 1: Example for the construction of the circuit given in Lemma A.1: a 4-colorable graph with maximum degree 3 alongside its associated depth-5 quantum circuit for the level-1 QAOA unitary.

B Optimal variational circuit for the ring of disagrees

In this section we consider the MaxCut Hamiltonian C on the cycle graph \mathbb{Z}_n . It is shown that the upper bound

$$\frac{1}{n} \langle +^n | U^\dagger C U | +^n \rangle \leq \frac{2p + 1/2}{2p + 1}.$$

established in the main text for any \mathbb{Z}_2 -symmetric range- p unitary U with $p < n/4$ is tight whenever n is an even multiple of $2p + 1$. Let

$$|\text{GHZ}_n\rangle = 2^{-1/2}(|0^n\rangle + |1^n\rangle)$$

be the GHZ state of n qubits.

Lemma B.1. *Suppose $n = 2p + 1$ for some integer p . There exists a \mathbb{Z}_2 -symmetric range- p quantum circuit V such that*

$$|\text{GHZ}_n\rangle = V|+^n\rangle. \quad (1)$$

Proof. We shall write $\text{CX}_{c,t}$ for the CNOT gate with a control qubit c and a target qubit t . Let H_j be the Hadamard gate acting on the j -th qubit and $c = p + 1$ be the central qubit. One can easily check that

$$|\text{GHZ}_n\rangle = \left(\prod_{j=1}^p \text{CX}_{c,c-j} \text{CX}_{c,c+j} \right) H_c |0^n\rangle.$$

All CX gates in the product pairwise commute, so the order does not matter. Inserting a pair of Hadamards on every qubit $j \in [n] \setminus \{c\}$ before and after the respective CX gate and using the identity $(I \otimes H)\text{CX}(I \otimes H) = \text{CZ}$ one gets

$$|\text{GHZ}_n\rangle = \left(\prod_{j \in [n] \setminus \{c\}} H_j \right) \left(\prod_{j=1}^p \text{CZ}_{c,c-j} \text{CZ}_{c,c+j} \right) |+^n\rangle. \quad (2)$$

Let $S = \exp[i(\pi/4)Z]$ be the phase-shift gate. Define the two-qubit Clifford gate

$$\text{RZ} = (S \otimes S)^{-1} \text{CZ} = \exp(-i\pi/4) \exp[-i(\pi/4)(Z \otimes Z)].$$

Expressing CZ in terms of RZ and S in Eq. (2) one gets

$$|\text{GHZ}_n\rangle = S_c^{2p} \left(\prod_{j \in [n] \setminus \{c\}} H_j S_j \right) \left(\prod_{j=1}^p \text{RZ}_{c,c-j} \text{RZ}_{c,c+j} \right) |+\rangle^n. \quad (3)$$

Multiply both sides of Eq. (3) on the left by a product of S gates over qubits $j \in [n] \setminus \{c\}$. Noting that

$$SHS = i \exp[-i(\pi/4)X]$$

one gets (ignoring an overall phase factor)

$$\prod_{j \in [n] \setminus \{c\}} S_j |\text{GHZ}_n\rangle = S_c^{2p} \left(\prod_{j \in [n] \setminus \{c\}} \exp[-i(\pi/4)X_j] \right) \left(\prod_{j=1}^p \text{RZ}_{c,c-j} \text{RZ}_{c,c+j} \right) |+\rangle^n. \quad (4)$$

Using the identity

$$\prod_{j \in [n] \setminus \{c\}} S_j |\text{GHZ}_n\rangle = S_c^{2p} |\text{GHZ}_n\rangle.$$

one can cancel S_c^{2p} that appears in both sides of Eq. (4). We arrive at Eq. (1) with

$$V = \left(\prod_{j \in [n] \setminus \{c\}} \exp[-i(\pi/4)X_j] \right) \left(\prod_{j=1}^p \text{RZ}_{c,c-j} \text{RZ}_{c,c+j} \right)$$

The circuit diagram of V in the case $n = 7$ is shown in Figure 2. Obviously, V is \mathbb{Z}_2 -symmetric since any individual gate commutes with $X^{\otimes n}$. Let us check that V has range- p . Consider any single-qubit observable O_q acting on the q -th qubit. Consider three cases. *Case 1:* $q = c$. Then $V^\dagger O_q V$ may be supported on all n qubits. However, $[c-p, c+p] = [1, n]$, so the p -range condition is satisfied trivially. *Case 2:* $1 \leq q < c$. Then all gates $\text{RZ}_{c,c+j}$ in V cancel the corresponding gates in V^\dagger , so that $V^\dagger O_q V$ has support in the interval $[1, c] \subseteq [q-p, q+p]$. Thus the p -range condition is satisfied. *Case 3:* $c < q \leq n$. This case is equivalent to Case 2 by symmetry. \square

Recall that the ring of disagrees Hamiltonian has the form

$$C = \frac{1}{2} \sum_{j \in \mathbb{Z}_n} (I - Z_j Z_{j+1}).$$

Lemma B.2. *Consider any integers n, p such that n is even and n is a multiple of $2p + 1$. Then there exists a \mathbb{Z}_2 -symmetric range- p circuit U such that*

$$\frac{1}{n} \langle +^n | U^\dagger C U | +^n \rangle = \frac{2p + 1/2}{2p + 1}.$$

Proof. Let W be the \mathbb{Z}_2 -symmetric range- p unitary operator preparing the GHZ state on $2p + 1$ qubits starting from $|+^{2p+1}\rangle$, see Lemma B.1. Suppose $n = m(2p + 1)$ for some even integer m . Define

$$U = \bar{X} W^{\otimes m},$$

where

$$\bar{X} = (X \otimes I)^{\otimes n/2}.$$

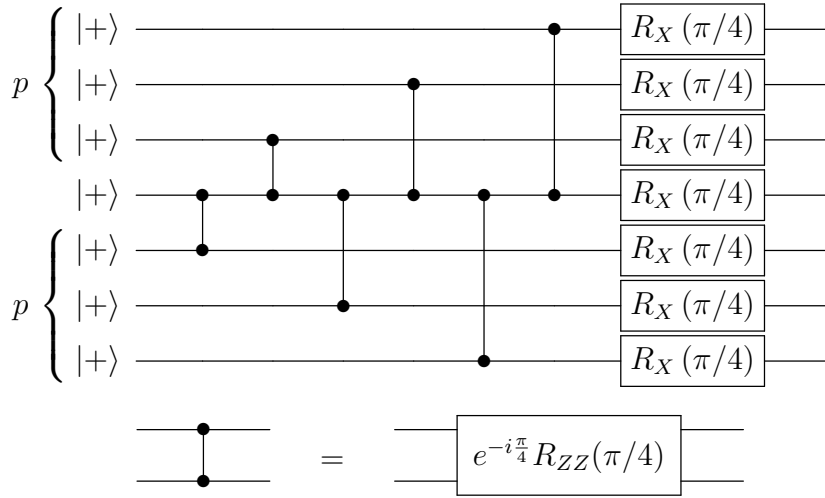


Figure 2: The \mathbb{Z}_2 -symmetric range-3 quantum circuit to prepare the GHZ state $|\text{GHZ}_{2p+1}\rangle$ of $2p+1 = 7$ qubits ($p = 3$). Here, $R_O(\theta) = \exp(-i\theta O)$.

Since each copy of W acts on a consecutive interval of qubits and has range p , one infers that U has range p . We have

$$\bar{X}^\dagger C \bar{X} = \sum_{k \in \mathbb{Z}_n} G_k, \quad \text{where} \quad G_k = \frac{1}{2}(I + Z_k Z_{k+1}).$$

The state $W^{\otimes m}|+^n\rangle$ is a tensor product of GHZ states supported on consecutive tuples of $2p+1$ qubits. The expected value of G_k on the state $W^{\otimes m}|+^n\rangle$ equals 1 if G_k is supported on one of the GHZ states. Otherwise, if G_k crosses the boundary between two GHZ states, the expected value of G_k on the state $W^{\otimes m}|+^n\rangle$ equals $1/2$. Thus

$$\langle +^n | U^\dagger C U | +^n \rangle = \sum_{k \in \mathbb{Z}_n} \langle +^n | (W^{\otimes m})^\dagger G_k W^{\otimes m} | +^n \rangle = m(2p+1/2) = n \left(\frac{2p+1/2}{2p+1} \right).$$

□

C Numerical simulation of level-1 QAOA and RQAOA

In this section we provide details of the simulation reported on Figure 1 in the main text. Let J be a real symmetric matrix of size n . Consider an Ising-type Hamiltonian

$$C = \sum_{1 \leq j < k \leq n} J_{j,k} Z_j Z_k.$$

Here $J_{j,k}$ are arbitrary real coefficients. Below we show how to compute the mean value of a Pauli operator $Z_j Z_k$ on the level-1 QAOA state

$$|\psi(\beta, \gamma)\rangle = e^{i\beta B} e^{i\gamma C} | +^n \rangle$$

in time $O(n)$ using an explicit analytic formula. Such a formula was derived for the MaxCut cost function by Wang et al. [27, Theorem 1]. Here we provide a generalization to arbitrary Ising

Hamiltonians. Since the total number of terms in the cost function is $O(n^2)$, simulating each step of RQAOA takes time at most $O(n^3)$. Assuming that $n_c = O(1)$, the number of steps is roughly n so that the full simulation cost is $O(n^4)$. Crucially, the simulation cost of this method does not depend on the depth of the variational circuit. This is important because RQAOA may potentially increase the depth from $O(1)$ to $O(n)$ since it adds many new terms to the cost function.

Lemma C.1. *Fix a pair of qubits $1 \leq j < k \leq n$. Let $c = \cos(2\beta)$ and $s = \sin(2\beta)$. Then*

$$\begin{aligned} \langle \psi(\beta, 1) | Z_j Z_k | \psi(\beta, 1) \rangle &= (s^2/2) \prod_{p \neq j, k} \cos[2J_{j,p} - 2J_{k,p}] - (s^2/2) \prod_{p \neq j, k} \cos[2J_{j,p} + 2J_{k,p}] \\ &\quad + cs \cdot \sin(2J_{j,k}) \left[\prod_{p \neq j, k} \cos(2J_{j,p}) + \prod_{p \neq j, k} \cos(2J_{k,p}) \right]. \end{aligned} \quad (5)$$

Here we only consider the case $\gamma = 1$ since γ can be absorbed into the definition of J .

Proof. Given a 2-qubit observable O define the mean value

$$\mu(O) = \langle \psi(\beta, 1) | O_{j,k} | \psi(\beta, 1) \rangle.$$

We are interested in the observable $O = ZZ \equiv Z \otimes Z$.

We note that all terms in B and C that act trivially on $\{j, k\}$ do not contribute to $\mu(O)$. Such terms can be set to zero. Given a 2-qubit observable O , define a mean value

$$\mu'(O) = \langle +^n | e^{iC'} O_{j,k} e^{-iC'} | +^n \rangle, \quad \text{where} \quad C' = \sum_{p \neq j, k} (J_{j,p} Z_j + J_{k,p} Z_k) Z_p. \quad (6)$$

Using the identities

$$\begin{aligned} e^{i\beta(X_j + X_k)} Z_j Z_k e^{-i\beta(X_j + X_k)} &= c^2 Z_j Z_k + s^2 Y_j Y_k + cs(Z_j Y_k + Y_j Z_k), \\ e^{iJ_{j,k} Z_j Z_k} Z_j Z_k e^{-iJ_{j,k} Z_j Z_k} &= Z_j Z_k, \\ e^{iJ_{j,k} Z_j Z_k} Y_j Y_k e^{-iJ_{j,k} Z_j Z_k} &= Y_j Y_k \\ e^{iJ_{j,k} Z_j Z_k} Z_j Y_k e^{-iJ_{j,k} Z_j Z_k} &= \cos(2J_{j,k}) Z_j Y_k + \sin(2J_{j,k}) X_k, \\ e^{iJ_{j,k} Z_j Z_k} Y_j Z_k e^{-iJ_{j,k} Z_j Z_k} &= \cos(2J_{j,k}) Y_j Z_k + \sin(2J_{j,k}) X_j, \end{aligned}$$

and noting that $\mu'(ZZ) = 0$ one easily gets

$$\mu(ZZ) = s^2 \cdot \mu'(YY) + cs \cdot \cos(2J_{j,k}) [\mu'(ZY) + \mu'(YZ)] + cs \cdot \sin(2J_{j,k}) [\mu'(XI) + \mu'(IX)]. \quad (8)$$

Using the explicit form of C' one gets

$$e^{-iC'} | +^n \rangle = \frac{1}{2} \sum_{a, b=0,1} |a, b\rangle_{j,k} \otimes |\Phi(a, b)\rangle_{\text{else}}, \quad (9)$$

where $|\Phi(a, b)\rangle$ is a tensor product state of $n - 2$ qubits defined by

$$|\Phi(a, b)\rangle = \bigotimes_{p \neq j, k} |J_{j,p}(-1)^a + J_{k,p}(-1)^b\rangle_p \quad \text{where} \quad |\theta\rangle \equiv e^{-i\theta Z} |+\rangle.$$

Combining Eqs. (6),(9) one gets

$$\mu'(O) = (1/4) \sum_{a, b, a', b'=0,1} \langle a', b' | O | a, b \rangle \cdot \langle \Phi(a', b') | \Phi(a, b) \rangle. \quad (10)$$

Using the tensor product form of the states $|\Phi(a, b)\rangle$ and the identity $\langle \theta' | \theta \rangle = \cos(\theta - \theta')$ gives

$$\langle \Phi(a', b') | \Phi(a, b) \rangle = \prod_{p \neq j, k} \cos [J_{j,p}(-1)^a - J_{j,p}(-1)^{a'} + J_{k,p}(-1)^b - J_{k,p}(-1)^{b'}]. \quad (11)$$

From Eqs. (10),(11) one can easily compute the mean value $\mu'(O)$ for any 2-qubit observable.

Consider first the case $O = YY$. Then the only terms contributing to Eq. (10) are those with $a' = a \oplus 1$ and $b' = b \oplus 1$. The identity $\langle a \oplus 1 | Y | a \rangle = -i(-1)^a$ gives

$$\mu'(YY) = -(1/4) \sum_{a,b=0,1} (-1)^{a+b} \prod_{p \neq j, k} \cos [2J_{j,p}(-1)^a + 2J_{k,p}(-1)^b],$$

that is,

$$\mu'(YY) = (1/2) \prod_{p \neq j, k} \cos [2J_{j,p} - 2J_{k,p}] - (1/2) \prod_{p \neq j, k} \cos [2J_{j,p} + 2J_{k,p}]. \quad (12)$$

Next consider the case $O = YZ$. Note that the matrix elements $\langle a', b' | O | a, b \rangle$ have zero real part. From Eqs. (10),(11) one infers that $\mu'(YZ)$ has zero real part. This implies

$$\mu'(YZ) = \mu'(ZY) = 0. \quad (13)$$

Finally, consider the case $O = XI$. Then the only terms that contribute to Eq. (10) are those with $a' = a \oplus 1$ and $b' = b$. We get

$$\mu'(XI) = \prod_{p \neq j, k} \cos (2J_{j,p}). \quad (14)$$

Here we noted that the inner product Eq. (11) with $a' = a \oplus 1$ and $b' = b$ does not depend on a, b . By the same argument,

$$\mu'(IX) = \prod_{p \neq j, k} \cos (2J_{k,p}). \quad (15)$$

Combining Eq. (8) and Eqs. (12),(13),(14),(15) one arrives at Eq. (5). \square

Clearly, the ability to simulate level-1 RQAOA with Ising-type cost functions on a classical computer in polynomial time precludes exponential quantum speedups. However, as far as we know, higher-level RQAOA with $p \geq 2$ lacks efficient classical simulation leaving room for a quantum advantage.

D RQAOA optimally solves the ring of disagrees

In this section we prove that the level-1 RQAOA optimally solves the ring of disagrees model. This is in sharp contrast to the standard QAOA which achieves approximation ratio at most $(2p+1)/(2p+2)$ for any level p , as was shown in Ref. [22]. More generally, we show that the level-1 RQAOA optimally solves any 1D Ising model where the coupling coefficients are either $+1$ or -1 .

Lemma D.1. *Consider a cost function*

$$C(x) = \sum_{k \in \mathbb{Z}_n} J_k (-1)^{x_k + x_{k+1}}$$

with n variables $x \in \{0, 1\}^n$ located at vertices of the cycle graph \mathbb{Z}_n . Assume that $J_k \in \{1, -1\}$ for all $k \in \mathbb{Z}_n$. Then the level-1 RQAOA outputs $x^* \in \{0, 1\}^n$ such that $C(x^*) = \max_x C(x)$.

Proof. Let

$$C = \sum_{k \in \mathbb{Z}_n} J_k Z_k Z_{k+1} \quad (16)$$

be the corresponding Hamiltonian. First, we observe that $\langle \psi(\beta, \gamma) | Z_i Z_j | \psi(\beta, \gamma) \rangle = 0$ if $\text{dist}(i, j) > 2$ since in this case the operators $U^{-1} Z_i U$ and $U^{-1} Z_j U$ have disjoint support. Lemma C.1 shows that

$$\langle \psi(\beta, \gamma) | Z_i Z_j | \psi(\beta, \gamma) \rangle = \begin{cases} \frac{1}{2} J_i \sin(4\beta) \sin(4\gamma) & \text{if } j = i + 1 \\ \frac{1}{4} J_i J_{i+1} \sin^2(2\beta) \sin^2(4\gamma) & \text{if } j = i + 2 \\ 0 & \text{otherwise} \end{cases} \quad (17)$$

when $J_k \in \{1, -1\}$ for every $k \in \mathbb{Z}_n$. Here we assumed $i < j$. Thus

$$|\langle \psi(\beta, \gamma) | Z_i Z_{i+2} | \psi(\beta, \gamma) \rangle| \leq 1/4 \quad (18)$$

for all β, γ . Let β^*, γ^* be the optimal angles maximizing the variational energy $\langle \psi(\beta, \gamma) | C | \psi(\beta, \gamma) \rangle$. Then we can infer from Eq. (17) that

$$\langle \psi(\beta^*, \gamma^*) | Z_i Z_{i+1} | \psi(\beta^*, \gamma^*) \rangle = J_i/2. \quad (19)$$

Combined with Eq. (17) and Eq. (18) we conclude that the maximally correlated pair of variables are nearest neighbors, that is,

$$\arg \max_{(i,j):i<j} |\langle \psi(\beta^*, \gamma^*) | Z_i Z_j | \psi(\beta^*, \gamma^*) \rangle| = (i^*, i^* + 1) \quad (20)$$

for some $i^* \in \mathbb{Z}_n$. Without loss of generality, assume that $i^* = n-2$. Then, according to Eq. (20), the RQAOA algorithm eliminates the variable Z_{n-1} . By Eq. (19), the corresponding parity constraint is

$$Z_{n-1} = Z_{n-2} J_{n-2}. \quad (21)$$

The resulting reduced graph obtained from \mathbb{Z}_n by contracting the edge $(n-1, n-2)$ is isomorphic to \mathbb{Z}_{n-1} . It is easy to check that the new cost function Hamiltonian C' acting on $n-1$ qubits is

$$C' = 1 + \sum_{k \in \mathbb{Z}_{n-1}} J'_k Z_k Z_{k+1} \quad (22)$$

with

$$J'_i = \begin{cases} J_i & \text{if } i \neq n-2 \\ J_{n-2} J_{n-1} & \text{if } i = n-2 \end{cases} \quad (23)$$

We note that the transformation Eq. (23) preserves the parity of the couplings in the sense that

$$\prod_{k \in \mathbb{Z}_n} J_k = \prod_{k \in \mathbb{Z}_{n-1}} J'_k. \quad (24)$$

Proceeding inductively, one eliminates variables $Z_{n-1}, Z_{n-2}, \dots, Z_{n_c}$ while imposing parity constraints (cf. Eq. (21))

$$\begin{aligned} Z_{n-1} &= Z_{n-2} J_{n-2} \\ Z_{n-2} &= Z_{n-3} J'_{n-3} \\ &\vdots \end{aligned}$$

arriving at the cost function Hamiltonian C'' for an Ising chain of length n_c having couplings ± 1 . Because of Eq. (24) and because the Hamiltonian Eq. (16) is frustrated if and only if $\prod_{k \in \mathbb{Z}_n} J_k = -1$, we conclude that any maximum $x^* \in \{0, 1\}^{n_c}$ of $C''(x)$ satisfies

$$C''(x^*) = \begin{cases} n_c & \text{if } \prod_{k \in \mathbb{Z}_{n_c}} J_k = 1 \\ n_c - 2 & \text{if } \prod_{k \in \mathbb{Z}_{n_c}} J_k = -1. \end{cases}$$

Because the cost function acquires a constant energy shift in every variable elimination, see Eq. (22), the final output x of the RQAOA algorithm satisfies

$$C(x) = n - n_c + C''(x^*) = \begin{cases} n & \text{if } \prod_{k \in \mathbb{Z}_n} J_k = 1 \\ n - 2 & \text{if } \prod_{k \in \mathbb{Z}_n} J_k = -1. \end{cases}$$

This implies the claim. □

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