Letter

Efficient quantum algorithm for solving structured problems via multistep quantum computation

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In classical computation, a problem can be solved in multiple steps where the calculated results of each step can be copied and used repeatedly. However, in quantum computation, it is difficult to realize a similar multistep computation process because the no-cloning theorem forbids making copies of an unknown quantum state perfectly. We find a method based on a quantum resonant transition to protect and reuse an unknown quantum state that encodes the calculated results of an intermediate step without copying it, and present a quantum algorithm that solves a problem via multistep quantum computation. We demonstrate that this algorithm can solve a type of structured search problems efficiently.

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Introduction. Solving a problem on a quantum computer can be transformed to finding the ground state of a problem Hamiltonian that encodes the solution to the problem. The phase estimation algorithm (PEA) [1,2] projects an initial state onto the ground state of the problem Hamiltonian with probability proportional to the square of the overlap between them. However, it is difficult to find a good initial state for a complicated system. By using amplitude amplification, quantum algorithms can achieve a quadratic speedup over classical algorithms in preparing the ground state of a quantum many-body system [3]. In adiabatic quantum computing (AQC) [4], a system is evolved adiabatically from the ground state of an initial Hamiltonian to that of the problem Hamiltonian. The efficiency of AQC depends on the minimum energy gap between the ground and the first excited states of the adiabatic Hamiltonian, which is difficult to estimate in most cases. The quantum Zeno effect [5,6] can be used to keep a quantum computer near the ground state of a smoothly varying Hamiltonian by performing frequent measurements, and has the same efficiency as AQC.

The structure of a problem is the key for whether or not it can be solved efficiently on a quantum computer. In Refs. [7,8], a nested search algorithm was proposed for problems that can be divided into two (or more) levels described by a set of primary and secondary variables, respectively. It works by nesting one quantum search within another, and performing a quantum search at a selected level among partial solutions to narrow the subsequent search over their descendants. The complete solution is constructed through a tree of partial solutions at different levels. This algorithm achieves quadratic speedup over the corresponding classical nesting algorithms, and can be faster than the usual Grover bound for an unstructured search. In general, the constraints of a problem contain variables that are coupled to each other, and the variables may be divided into only a few sets, thus the search space is still exponentially large.

In the circuit model, a quantum computation is performed by first preparing qubits in an initial state, then applying a series of unitary operations, and finally measuring the qubits to obtain the calculation results. However, in classical computation, a problem can be solved in multiple steps. In each step, with the calculated results of the previous step as input, one performs a calculation, then checks if the results satisfy certain conditions; if the conditions are satisfied, then the calculation of the next step is continued; otherwise, the procedure is repeated iteratively until the desired results are obtained. This process is easy to implement in classical computation since the results of each step can be copied and used repeatedly, and the runtime is proportional to the number of steps. In quantum computation, however, it is difficult to realize a similar multistep quantum computation process due to the restriction of the no-cloning theorem [9,10], which forbids making copies of an unknown quantum state perfectly. Calculated results encoded in an unknown quantum state cannot be used by making copies as in classical computation. Therefore in multistep quantum computation, if one fails to obtain the desired results of a step, one has to run the algorithm from the beginning again. This leads to the result that

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TABLE I. Comparison of the performance of some algorithms for solving the structured search problem. The AQC algorithm and the Grover's algorithm use the same Hamiltonian evolution path as our algorithm. The performance of the method in Ref. [5] is the same as that of the AQC algorithm. The term N represents the dimension of the search space.

Algorithms	Runtime	Determining factors
AQC	$O(N^2)$	Minimum energy gap between the ground and the first excited states of each adiabatic evolution Hamiltonian
Grover	$O(\sqrt{N})$	Query number of the oracles
PEA	$O(N)$	Overlap between a guess state and the ground state of the problem Hamiltonian
Our algorithm	$O(\log N)$	Ratio N_j/N_{j-1}; here, N_j represents the number of marked states of the jth step

the runtime scales exponentially with the number of steps of the algorithm, since the success probability of the algorithm is the product of the success probability in each step.

We find a method to protect and reuse an unknown quantum state that encodes the calculated results of an intermediate step without copying it. Using this method, we present a quantum algorithm for finding the ground state of a problem Hamiltonian via multistep quantum computation, and apply it to efficiently solve a type of structured search problems that can be decomposed in a more general way than that in Refs. [7,8], so the search space of the problems is reduced in polynomial rate to the target state, while it is difficult to solve them through the usual quantum computation process.

The idea of the algorithm is as follows: We construct an evolution path from an initial Hamiltonian H_0 to a problem Hamiltonian H_P by inserting between them a sequence of intermediate Hamiltonians $\{H_l, l = 1, \ldots, m-1\}$, through which H_0 reaches H_P as $H_0 \to H_1 \to \cdots \to H_{m-1} \to H_P = H_m$. We start from the ground state $|\varphi_0^{(0)}\rangle$ of H_0, and evolve it through ground states of the intermediate Hamiltonians sequentially to the ground state $|\varphi_0^{(m)}\rangle$ of H_P in m steps. In each step, the ground state of an intermediate Hamiltonian is obtained deterministically via quantum resonant transitions (QRTs) [11,12]. For simulatable Hamiltonians, i.e., Hamiltonians that can be simulated efficiently on a quantum computer, our algorithm can be run efficiently if (i) the overlaps between the ground states of any two adjacent Hamiltonians and (ii) the energy gap between the ground and the first excited states of each Hamiltonian are not exponentially small. The conditions can be reduced to simpler forms for problems with special structures.

With the property of being able to solve a problem via multistep quantum computation, our algorithm can solve a problem efficiently even when the overlap between an initial state and the solution state of the problem Hamiltonian is exponentially small, as long as the above conditions are satisfied. The success probability of the PEA is exponentially small in this case. We demonstrate that our algorithm can solve a type of structured search problems efficiently, while the usual AQC algorithm (the adiabatic evolution Hamiltonian is set as a linear interpolation of an initial and a final Hamiltonians), which has the same efficiency as the algorithm in Ref. [5], cannot solve this problem efficiently. The AQC can achieve the same efficiency as our algorithm with a jagged adiabatic path [13]. We summarize the performance of the algorithms for solving the structured search problems in Table I and provide details in Sec. VI of the Supplemental Material (SM) [14].

The algorithm. We describe the algorithm by using one of its steps as an example. By optimizing the algorithm in Refs. [11,12], one qubit is saved in this algorithm. For a problem of dimension $N = 2^n$, the algorithm requires $(n+1)$ qubits with one probe qubit and an n-qubit register R representing the problem. In the lth step, given the Hamiltonians H_l, H_{l-1} and its ground state $|\varphi_0^{(l-1)}\rangle$ prepared on the register R and the corresponding eigenvalue $E_0^{(l-1)}$ obtained from previous step, we aim to prepare the ground state $|\varphi_0^{(l)}\rangle$ and obtain the corresponding eigenvalue $E_0^{(l)}$ of H_l. The algorithm Hamiltonian of the lth step is

$$H^{(l)} = -\tfrac{1}{2}\omega\sigma_z \otimes I_N + H_R^{(l)} + c\sigma_x \otimes I_N, \tag{1}$$

where

$$H_R^{(l)} = \alpha_l |1\rangle\langle 1| \otimes H_{l-1} + |0\rangle\langle 0| \otimes H_l, \quad l = 1, 2, \ldots, m, \tag{2}$$

I_N is the N-dimensional identity operator, and σ_x, σ_z are the Pauli matrices. The first term in Eq. (1) is the Hamiltonian of the probe qubit, the second term contains the Hamiltonian of the register R and describes the interaction between the probe qubit and R, and the third term is a perturbation. The parameter α_l is used to rescale the energy levels of H_{l-1}, and the ground-state energy of $\alpha_l H_{l-1}$ is used as a reference point to the ground-state eigenvalue of H_l, and $c \ll 1$. We estimate the range of the ground-state eigenvalue $E_0^{(l)}$ of H_l and obtain the estimated transition frequency range $[\omega_{\min}, \omega_{\max}]$ between states $|\varphi_0^{(l-1)}\rangle$ and $|\varphi_0^{(l)}\rangle$. Then we discretize the frequency range into a number of grids and use them as detection frequencies of the probe qubit. Procedures for the lth step of the algorithm are as follows:

(i) Set the probe qubit in a frequency from the frequency set, and initialize it in its excited state $|1\rangle$ and the register R in state $|\varphi_0^{(l-1)}\rangle$.

(ii) Implement the time evolution operator $U(t) = \exp(-iH^{(l)}t)$ for a time t determined by the overlap between the states $|\varphi_0^{(l-1)}\rangle$ and $|\varphi_0^{(l)}\rangle$ (see Sec. I of SM [14]).

(iii) Read out the state of the probe qubit.

We repeat procedures (ii) and (iii) a number of times. If the measurement on the probe qubit results in state $|1\rangle$, it indicates that the register R remains in the state $|\varphi_0^{(l-1)}\rangle$, and then we run procedures (ii) and (iii) by setting the probe qubit in another frequency. Otherwise, if the probe qubit decays to state $|0\rangle$, it indicates a resonant transition from state $|1\rangle|\varphi_0^{(l-1)}\rangle$ to $|0\rangle|\varphi_0^{(l)}\rangle$ has occurred. The eigenvalue $E_0^{(l)}$ of H_l can be obtained by locating the resonant transition frequency of the probe qubit that satisfies $E_0^{(l)} - \alpha_l E_0^{(l-1)} = \omega$

(see Sec. I of SM [14]). The corresponding eigenvector $|\varphi_0^{(l)}\rangle$ can be prepared by running the above procedure at the resonant transition frequency [11,12]. With H_l, $|\varphi_0^{(l)}\rangle$, and $E_0^{(l)}$, we run the algorithm for the next step. Proceeding step by step, finally we obtain the ground state of the problem Hamiltonian. For some problems, the ground-state eigenvalues of the intermediate Hamiltonians can be calculated analytically, therefore the implementation of the algorithm becomes easier.

As the resonant transition occurs, the system is approximately in a state $\sqrt{1-p_0^{(l)}}|1\rangle|\varphi_0^{(l-1)}\rangle + \sqrt{p_0^{(l)}}|0\rangle|\varphi_0^{(l)}\rangle$, where $p_0^{(l)} = \sin^2(ctd_0^{(l)})$ is the decay probability of the probe qubit of the lth step, and $d_0^{(l)} = \langle\varphi_0^{(l-1)}|\varphi_0^{(l)}\rangle$. The state $|\varphi_0^{(l-1)}\rangle$ is protected in this entangled state. If the measurement outcome on the probe is in state $|0\rangle$, it indicates the state $|\varphi_0^{(l)}\rangle$ is obtained on the register R, and then we run the $(l+1)$th step of the algorithm. Otherwise, if the probe is in state $|1\rangle$, it means R remains in the state $|\varphi_0^{(l-1)}\rangle$, and we repeat the procedures (ii) and (iii) by setting the probe in the resonant transition frequency until it decays to state $|0\rangle$. By protecting the calculated result of an intermediate step in this entangled state, we do not need to run the algorithm from the beginning once it fails to obtain the desired state in a step of the algorithm. We just repeat the procedures of the step until the desired state is obtained. With this property, the desired state of each step is obtained deterministically in polynomial time if the conditions of the algorithm are satisfied. Here, "deterministically" means that by running the procedures of a step repeatedly, we know exactly when the desired state of the step is obtained from the measurement outcome on the probe qubit. The number of times the procedures have to be repeated is proportional to $1/p_0^{(l)}$. Therefore, the runtime of the algorithm is proportional to $\sum_{l=1}^{m} 1/p_0^{(l)}$, which scales linearly with the number of steps of the algorithm, provided $p_0^{(l)}$ are not exponentially small in the system size n.

There are various ways to construct evolution paths that satisfy the conditions of the algorithm. Here, we present two methods: (i) For a system Hamiltonian $H_0 + V$, by writing $H = H_0 + gV$ $(g \in [0,1])$ and discretizing the parameter g, the intermediate Hamiltonians can be constructed as $H_l = H_0 + g_l V$ $(0 = g_0 < g_1 < \cdots < g_m = 1)$ [6]. The parameters g_l can be adjusted to make $d_0^{(l)}$ finite. (ii) The system Hamiltonian can be a Hamiltonian matrix, and intermediate Hamiltonian matrices can be constructed by spanning the system Hamiltonian in a sequence of basis sets with increasing dimension such that the matrix H_{l-1} is contained in a subspace of the adjacent matrix H_l. The dimension of the basis sets can be adjusted to make $d_0^{(l)}$ finite. The path can also be constructed by considering the structure of the problem.

In the lth step, the probability of the initial state being evolved to the state $|0\rangle|\varphi_0^{(l)}\rangle$ reaches maximum at $t = \pi/(2cd_0^{(l)})$. Errors are introduced as the initial state leaks to the excited states $|0\rangle|\varphi_j^{(l)}\rangle$ $(j = 1, \ldots, N-1)$ with probability p_j. By assuming $E_1^{(l)} - E_0^{(l)} \gg cd_0^{(l)}$ and $\alpha_l(E_1^{(l-1)} - E_0^{(l-1)}) \gg cd_0^{(l)}$, and setting the optimal runtime $t = \pi/(2cd_0^{(l)})$ for convenience, we have

$$\sum_j p_j \leqslant a_l^2 c^2, \tag{3}$$

where

$$a_l^2 = \frac{4\left[1-\left(d_0^{(l)}\right)^2\right]}{\left[E_1^{(l)} - E_0^{(l)}\right]^2}.$$

(see Sec. I of SM [14]). If the energy gaps $E_1^{(l)} - E_0^{(l)}$ are not exponentially small, i.e., bounded by a polynomial function of the problem size, then a_l is finite and the error in the lth step is bounded by $a_l^2 c^2$. Considering errors accumulated in all steps, the success probability of the algorithm satisfies

$$P_{\text{succ}} \geqslant \prod_{l=1}^{m}\left[1 - a_l^2 c^2\right] \geqslant [1 - (a_{\max} c)^2]^m,$$

where $a_{\max}$ is the maximum value of a_l (see Sec. I of SM [14]). The coefficient c can be set such that $a_{\max} c < 1/\sqrt{m}$, then $P_{\text{succ}} > 1/e$ in the asymptotic limit of m. The runtime of each step is proportional to $\pi/(2cd_0^{(l)})$, therefore the runtime of the algorithm scales as $O(\sum_{l=1}^{m} \frac{\pi}{2(E_1^{(l)} - E_0^{(l)})d_0^{(l)}})$.

The time evolution operators $U(t) = \exp(-iH^{(l)}t)$ can be implemented efficiently using Hamiltonian simulation algorithms [15,16]. Our algorithm requires performing single-qubit measurements and resetting the probe qubit to its excited state; such techniques have been realized in an ion-trap experiment [17]. We now apply the algorithm for solving a type of search problems with a special structure.

Search problem with a special structure. The unstructured search problem is to find a marked item in an unsorted database of N items using an oracle that recognizes the marked item. The oracle is defined in terms of a problem Hamiltonian $H_P = -|q\rangle\langle q|$, where $|q\rangle$ is the marked state associated with the marked item. The initial Hamiltonian is defined as $H_0 = -|\psi_0\rangle\langle\psi_0|$, where $|\psi_0\rangle = \frac{1}{\sqrt{N}}\sum_{j=0}^{N-1}|j\rangle$. We consider a search problem with a structure that can be decomposed by using m [in order of $O(\log N)$] oracles to construct a sequence of intermediate Hamiltonians

$$H_i = \frac{N_i}{N}H_0 + \left(1 - \frac{N_i}{N}\right)H_{P_i}, \quad i = 1, 2, \ldots, m-1, \tag{4}$$

where

$$H_{P_i} = -\sum_{q_i \in \Pi_i}|q_i\rangle\langle q_i|, \tag{5}$$

and $H_m = H_P$ and Π_m only contains the target state $|q\rangle$, and $\Pi_1 \supset \cdots \supset \Pi_{m-1} \supset \Pi_m$ with sizes $N_1, \ldots, N_{m-1}, N_m = 1$, respectively. If N_i/N_{i-1} $(i = 1, 2, \ldots, m)$ are not exponentially small, the problem can be solved efficiently in m steps by using our algorithm.

Define $|q_i^{\perp}\rangle = \frac{1}{\sqrt{N-N_i}}\sum_{j\notin\Pi_i}|j\rangle$. In the basis $(\{|q_i\rangle\}_{q_i\in\Pi_i}, |q_i^{\perp}\rangle)$, the Hamiltonian H_i in Eq. (4) can be

written as

$$H_i = \begin{pmatrix} \frac{\xi-1}{N} & \cdots & \frac{\xi-1}{N} & \frac{(\xi-1)\sqrt{N-N_i}}{N} \\ \vdots & \ddots & \vdots & \vdots \\ \frac{\xi-1}{N} & \cdots & \frac{\xi-1}{N} & \frac{(\xi-1)\sqrt{N-N_i}}{N} \\ \frac{(\xi-1)\sqrt{N-N_i}}{N} & \cdots & \frac{(\xi-1)\sqrt{N-N_i}}{N} & \xi^2 \end{pmatrix} - \xi I_{N_i+1}, \tag{6}$$

where $\xi = 1 - \frac{N_i}{N}$ and I_{N_i+1} is the identity matrix of dimension $N_i + 1$. The eigenvalues of the ground and the first excited states of H_i are $E_\pm^{(i)} = \frac{-1\pm\Delta E_i}{2}$, respectively, where $\Delta E_i = \sqrt{(1-\frac{2N_i}{N})^2 + 4\frac{N_i^2}{N^2}(1-\frac{N_i}{N})}$ is the energy gap between them and reaches minimum $\sqrt{11}/3\sqrt{3} \approx 0.638$ at $N_i/N = 1/3$. Let $\mathbf{e} = (1, \ldots, 1)^{\mathrm{T}}$ and $\mathbf{0} = (0, \ldots, 0)^{\mathrm{T}}$ be $N_i \times 1$ vectors, respectively, so there are $N_i - 1$ degenerate eigenstates $|e_i'\rangle = (|e_i^\perp\rangle, 0)^{\mathrm{T}}$ of H_i with an eigenvalue $-\xi$, where $|e_i^\perp\rangle$ is orthogonal to $\mathbf{e}$. These eigenstates are uncoupled from the ground and the first excited states of H_i [20]. The condition for a resonant transition between states $|1\rangle|V_-^{(i-1)}\rangle$ and $|0\rangle|V_-^{(i)}\rangle$ is satisfied by setting $\omega = 1$ and $\alpha_i = (E_-^{(i)} - 1)/E_-^{(i-1)}$. The ground state of H_i is $|V_-^{(i)}\rangle = x_1^{(i)}(\mathbf{e}, 0)^{\mathrm{T}} + x_2^{(i)}(\mathbf{0}, 1)^{\mathrm{T}}$. After normalization, the overlap between the ground states of two adjacent intermediate Hamiltonians is

$$d_0^{(i)} = \langle V_-^{(i-1)}|V_-^{(i)}\rangle = \sqrt{\frac{N_i}{N_{i-1}}} x_1^{(i-1)*} x_1^{(i)} + \frac{N_{i-1}-N_i}{\sqrt{N_{i-1}(N-N_i)}} x_1^{(i-1)*} x_2^{(i)} + \sqrt{\frac{N-N_{i-1}}{N-N_i}} x_2^{(i-1)*} x_2^{(i)}. \tag{7}$$

The components $x_1^{(i)}$ and $x_2^{(i)}$ are functions of N_i/N, and $x_1^{(i)}$ contributes most to $|V_-^{(i)}\rangle$. If the ratios N_i/N_{i-1} are finite, where $N_0 = N$, then $d_0^{(i)}$ are finite, and the conditions of our algorithm are satisfied. So the problem can be solved efficiently through the path in Eq. (4) by setting the optimal runtime in each step since $d_0^{(i)}$ can be calculated. The overlap between the ground states of H_i and H_P is proportional to $\frac{1}{\sqrt{N_i}}|x_1^{(i)}|$, which increases monotonically as H_i approaches H_P.

We find some problems have the structure described above [18]. As an example, we apply our algorithm to solve the Deutsch-Jozsa problem (see Sec. II of SM [14]). For the unstructured search problem with one marked item, only one oracle can be used to separate the marked item from the unmarked items, where the ratio of N_1/N_0 is $1/N$. Our algorithm has the same efficiency as that of the Grover's algorithm [19] and the AQC algorithm [20,21] in solving this problem (see Sec. III of SM [14]).

Comparison of the algorithm with adiabatic quantum computing. In our algorithm, the ground state of the problem Hamiltonian is induced step by step through QRTs following a path from the initial Hamiltonian to the problem Hamiltonian. It solves a type of structured search problems efficiently. Applying AQC for this problem with adiabatic Hamiltonian $H(s) = (1-s)H_0 + sH_P$, $s \in [0, 1]$, the minimum energy gap between the ground and the first excited states of $H(s)$ is $1/\sqrt{N}$ at $s = 1/2$, and the runtime scales as $O(\sqrt{N})$.

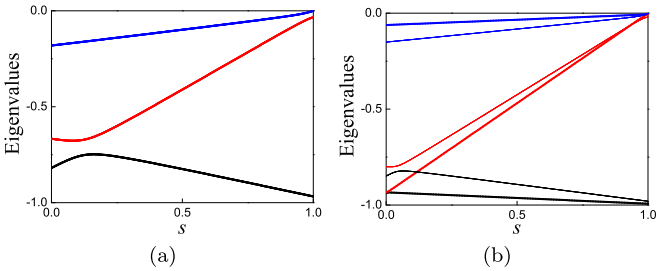

FIG. 1. Eigenvalue spectrum of the adiabatic Hamiltonian $H_i'(s)$ of an intermediate step with $N_i/N_{i-1} = 1/10$ vs the parameter s by setting the parameter N_i/N at different values. (a) $N_i/N = 1/30$; (b) the dashed thin lines represent the case $N_i/N = 1/50$, and the solid thick lines represent the case $N_i/N = 1/150$.

What about running AQC with the same path as our algorithm for solving this problem? We set N_i/N_{i-1} to be finite, thus the conditions of our algorithm are satisfied. Let the system evolve from the ground state of H_{i-1} to that of H_i under the adiabatic Hamiltonian $H_i'(s) = (1-s)H_{i-1} + sH_i$. We set $N_i/N_{i-1} = 1/10$ and calculate eigenvalues of $H_i'(s)$ for $1 < i < m$. In Fig. 1, we draw the energy spectrum of $H_i'(s)$ vs s where $0 < s < 1$ by setting $N_i/N = 1/30$, $1/50$, and $1/150$, respectively. As N_i/N becomes small, the minimum energy gap between the ground and the first excited states of $H_i'(s)$ decreases quickly as $s \to 0$, and scales as $O(1/N^2)$ at the asymptotic limit of N (see Sec. V of SM [14]). Thus the usual AQC algorithm cannot solve this problem efficiently using the path of our algorithm. The reason for this may be due to the structure coefficients N_i of the problem being used in constructing the intermediate Hamiltonians. It has been found that for an adiabatic path constructed in a linear interpolation of two Hamiltonians, the gaps can become superexponentially small, and the time for adiabatic evolution is longer than the time required for even a classical brute force search [13,22]. The AQC algorithm with a jagged adiabatic path [13] can have the same efficiency as our algorithm in solving the structured search problem. This approach requires one to project out the ground state of each Hamiltonian to form an adiabatic path. In comparison, our algorithm is much simpler, which needs only one ancilla qubit and its implementation requires only a Hamiltonian simulation for which there are optimal quantum algorithms [15,16] for simulatable Hamiltonians. In Table I, we list the performance of different algorithms for solving the structured search problem. Detailed comparisons are discussed in Sec. VI of SM [14].

Discussion. We present a quantum algorithm that solves a problem through multistep quantum computation in which an unknown quantum state that encodes the calculated results of an intermediate step can be protected and reused without copying it. The runtime is proportional to the number of steps of the algorithm, provided the conditions of the algorithm are satisfied. We find a type of search problems with a special structure can be solved efficiently by using our algorithm. Our algorithm provides another possibility for universal quantum computing and developing different quantum algorithms for other problems.

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[14] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevResearch.5.L012004 for The information of error analysis of the algorithm, application of the algorithm for solving the Deutsch-Jozsa problem and the unstructured search problem, application of Grover's algorithm and the quantum adiabatic algorithm for solving the search problem with a special structure, and a summary of the performance of different algorithms for solving the search problem with a special structure.

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