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Quantum thermal search: computing ground states via quantum mixing thermal operations

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The BBBV theorem is known to largely prohibit exponential speedup of quantum search over classical search, though not entirely, with potential loopholes such as adiabatic quantum computing. Recently, Chen-Huang-Preskill-Zhou (CHPZ) quantum (thermal) gradient descent proposal suggested another potential way to go around the BBBV theorem. We simplify the heavily complicated CHPZ analysis by focusing on the final equilibrium in the quantum thermal operation framework that has already been rigorously formulated in quantum thermodynamics, resulting in quantum thermal search. In particular, repeated applications of an identical quantum mixing thermal operation result in exponential convergence (in the number of repeated applications) of the system state to the equilibrium Gibbs state for the given system Hamiltonian at initial bath temperature. This allows for an efficient computation of the system ground state. Quantum mixing thermal operations evade the BBBV theorem by transferring initial system state information to the bath. Despite computational advantage of CHPZ and quantum thermal search for computing the ground state, it is also noted that some ground state computations corresponding to NP decision problems may require bath states that are exponentially close to the bath ground state, which translates to polynomially-scaling inverse bath temperature, potentially limiting usefulness of quantum thermal search. Potential implications for black hole physics, in light of pure to mixed and back to pure state evolution, are briefly noted.

1 Introduction

It is well-known that the BBBV theorem constrains how powerful quantum search can be over classical search [3]. Up to this point, Grover search [5, 11] is, for most of time, the best we can hope for within conventional quantum computing, with only quadratic speedup over classical search. Adiabatic quantum

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computing offers a potential way out of BBBV theorem restrictions [9], but it is believed that in most NP-complete-related instances, energy gap quickly becomes small such that computational advantages are largely lost.

As noted above, the BBBV theorem does not completely rule out loopholes, and most recently (late 2023 and early 2024), the Chen-Huang-Preskill-Zhou (CHPZ) quantum gradient descent method [7] has been proposed to (partially) evade such restrictions with thermal interactions. (Other examples involving thermality are there - see, as an example, [1].) From the point of system S in question, evolution is irreversible in CHPZ. However, if the universe remains in unitary evolution, then constraints of reversible unitary dynamics are still in place.

A major goal of this paper therefore is to provide an intuitive explanation as to why the CHPZ idea works without clashing with the BBBV theorem by utilizing the quantum thermal operation framework [4, 8] and resulting equilibration [6, 14] - via such an investigation, potential limitations and bounds of such computation ideas may be discovered.

Note that this paper largely shares the setup with CHPZ and adiabatic quantum computing (AQC) [9] in sense that we work with Hamiltonians that correspond to decision problems, instead of states corresponding to decision problems (Grover search). **Or more simply, the goal of quantum thermal search in this paper is to compute states close to the ground state of system Hamiltonian H_S , as with AQC.**

Also note that it is misguided to criticize CHPZ (and this paper) on the ground that 1) open quantum systems can still be simulated by a quantum algorithm and thus no advantage can be offered via thermodynamics - indeed, thermal operations [4] maintain reversible unitary evolution universe-wide, so this criticism is invalid from the start, 2) mixed initial states cannot offer much advantage over pure states in quantum computation - indeed, in case of zero-temperature baths with pure states as initial system states, the universe is always in a pure state under thermal operations.

The reason why CHPZ and quantum thermal search of this paper avoid the BBBV theorem and typical reversible unitarity constraints is explained in subsection 2.4. To state briefly, initial system state information is transferred to bath BH : while system S exponentially converges to the Gibbs state at initial bath temperature, BH equilibrates to different states depending on initial system states - no violation of

unitarity.

Potential limitations of quantum thermal search are explored in sub-subsection 2.6.2 and subsection 2.7 - under \tilde{n} repeated applications of an identical quantum mixing thermal operation in the large- \tilde{n} limit, it turns out that polynomially-scaling inverse bath temperature β_{BH} (relative to n , with 2^n being the system Hilbert space dimension) is necessary to obtain system states close to the ground state for some system Hamiltonians corresponding to NP decision problems. Polynomial scaling implies that the bath state has to be exponentially close to the bath ground state, which can turn out to be impractical.

In the conclusion, we also briefly examine how the equilibration process of mixing thermal operations in the $\tilde{n} \rightarrow \infty$ limit resembles something of black hole evaporation, in sense that system S can evolve from a pure state to a heavily mixed state, back to a pure state via cooling.

2 Quantum thermal search to find states close to the system ground state

2.1 Quantum thermal operations

Throughout this paper, it is assumed that interactions are of quantum mixing thermal operations [4, 8, 6, 14], though we first start with (general) quantum thermal operations and then justify ergodicity and more specifically, mixing properties in subsection 2.2.

Before defining quantum thermal operations mathematically, let us first outline the key properties of (quantum) thermal operations $\phi(\cdot, \gamma_{BH})$, where γ_{BH} is the bath Gibbs state (Equation (1)) at bath temperature T_{BH} for Hamiltonian H_{BH} [4, 8]:

1. One of their fixed point states is the Gibbs state γ_S for system S at bath temperature T_{BH} (Equation (3)). That is, $\phi(\gamma_S) = \gamma_S$. By restricting to quantum mixing thermal operations (subsection 2.2), the only fixed point that is a density matrix becomes γ_S , and in the $\tilde{n} \rightarrow \infty$ limit of applying same ϕ \tilde{n} times, the Gibbs state fixed point becomes the equilibrium state for system S [6, 14]. We may consider the $\tilde{n} \rightarrow \infty$ limit as the infinite-dimensional limit or the large bath limit.
2. Initial states of bath BH are Gibbs states γ_{BH} , as can be noticed in $\phi(\cdot, \gamma_{BH})$. No restriction is made to the initial state of system S .
3. They are unitary operations from the universe (system plus bath, $S + BH$) point of view. There-

fore, search procedures in either CHPZ [7] or this paper do not rely on non-unitary or irreversible operations for computational advantage.

4. Since thermal operations are unitary universe-wise, small perturbations to the initial *universe* state only induce small perturbations to the equilibrium *universe* state. If two initial system states are close, then in case one initial state quickly evolves to some equilibrium, then the other initial state has to evolve and converge quickly as well.

Let the universe consist of system S and bath BH , each with Hamiltonian H_S, H_{BH} . At initial time $t = 0$, bath BH is in Gibbs state γ_{BH} such that:

$$\gamma_{BH} = \frac{e^{-\beta_{BH}H_{BH}}}{\text{Tr}[e^{-\beta_{BH}H_{BH}}]} \quad (1)$$

Additionally, let the initial state of system S be $\rho_{S,init}$, and let $\beta_{BH} \equiv 1/k_B T_{BH}$ be the inverse temperature of BH , with T_{BH} being the temperature of BH . $\text{Tr}[\cdot]$ refers to trace.

A (quantum) thermal operation $\phi_{\gamma_{BH}, U_{SBH}} \equiv \phi$ (notation is simplified since the context is obvious) with some unitary U_{SBH} then goes as:

$$\begin{aligned} \phi(\cdot) &\equiv \text{Tr}_{BH} \left[U_{SBH}((\cdot) \otimes \gamma_{BH}) U_{SBH}^\dagger \right] \\ [U_{SBH}, H_S + H_{BH}] &= 0 \end{aligned} \quad (2)$$

where $\text{Tr}_{BH}[\cdot]$ refers to partial trace over bath BH . The second line of Equation (2) implies that the total non-interaction energy is conserved by a thermal operation. It is also known [4, 8] that $\phi(\gamma_S) = \gamma_S$ (the fixed-point property), where

$$\gamma_S = \frac{e^{-\beta_{BH}H_S}}{\text{Tr}[e^{-\beta_{BH}H_S}]} \quad (3)$$

2.2 Quantum mixing thermal operations

We now wish to impose that Gibbs state γ_S is the *unique* fixed point density matrix of ϕ - such a property is given by ergodicity [6, 14]. This eliminates other final equilibrium states.

For analytical simplicity without much loss of generality, we further assume that thermal operation

ϕ is a *mixing* quantum channel [6, 14]:

$$\lim_{\tilde{n} \rightarrow \infty} \|\phi^{\tilde{n}}(\rho) - \gamma_S\| = 0 \quad (4)$$

for all density operators ρ , where $\phi^{\tilde{n}}(\cdot) = [\phi \circ \phi \dots \circ \phi](\cdot)$. This mixing channel condition is satisfied (and thus does not require assuming), if the following assumption is satisfied (see Assumption 1 in [14]): there exists $N_0 \in \mathbb{N}$ such that for all $\tilde{n} > N_0$,

$$A > 0 \Rightarrow \phi^{\tilde{n}}(A) > 0 \quad (5)$$

As explained in [14], the assumption is satisfied as long as there is non-negligible decoherence ('mixing').

For mixing channel ϕ , the exponential suppression result is also known (see Theorem 1, Equation 3 of [14]):

$$\|\phi^{\tilde{n}}(\rho) - \gamma_S\| \leq c_x \mu^{\tilde{n}-1} \quad (6)$$

where c_x and μ are some constants. Note that μ can be determined from the infinite limit channel $\lim_{\tilde{n} \rightarrow \infty} \phi^{\tilde{n}}$, as seen in Equation A3 of [14] and that μ does not depend on the initial system state $\rho_{S,init}$.

With the unique fixed point γ_S confirmed for ϕ , and the output of $\phi^{\tilde{n}}$ well-approximated by γ_S , we now turn to the question of equilibration. From now on, we assume that ϕ is a quantum mixing thermal operation.

2.3 Equilibration via a large bath of \tilde{n} identical sub-baths

Two types of equilibration may be noted for mixing thermal operations:

- Equilibration toward the unique fixed point γ_S under repeated applications of ϕ as in Equation (6). This requires \tilde{n} copies of bath state γ_{BH} .
- Equilibration toward some equilibrium when interacting with a single sub-bath via universe Hamiltonian H (with $e^{-iHt} = U_{SBH}$, $\tilde{n} = 1$) for time duration t , as $t \rightarrow \infty$, with equilibration time analysis as suggested in [10].

We work with the first case since it is much simpler, but subsection 2.4 also provides one reason for this choice. Via the exponential error suppression result (relative to \tilde{n}) in Equation (6), the $\tilde{n} \rightarrow \infty$ limit may be utilized to simplify calculations without noticeable loss of validity and accuracy.

2.4 Non-applicability of the BBBV theorem for mixing thermal operations

It is beneficial to briefly consider why the BBBV theorem does not apply to mixing thermal operations. Mixing thermal operations work on the closed universe (in sense that its non-interaction energy is conserved and the von Neumann entropy of the universe is also conserved), so the open system is not the reason why the BBBV theorem is not applicable.

A mixed state of the universe is also not the reason why the BBBV theorem is not applicable, since some pure states are ground states, which are Gibbs states at zero temperature. Furthermore, there is no restriction for the initial state of system S . If the initial universe state is a pure state, then the universe is always in a pure state.

The zero-temperature example is quite useful, since it helps us clear a common misunderstanding. As $\tilde{n} \rightarrow \infty$, $\phi^{\tilde{n}}$ with zero-temperature BH has the system state converge to the zero-temperature Gibbs pure state, regardless of the initial system state $\rho_{S,init}$. Unitarity dictates that two very different initial pure states of the universe cannot evolve to similar pure states - thus, what changes is the bath state: initial system state information is ‘transferred’ to bath BH : the cost of system state convergence is state differences in BH . **This is a consequence of mixing thermal operations alone.**

The above also suggests that Gibbs state equilibration is one-sided in mixing thermal operations: system S loses its information to bath BH except initial bath temperature T_{BH} (which was not initial system information) and system Hamiltonian H_S , but bath BH could equilibrate to a non-Gibbs final state. The reason why the one-sided transformation is possible has to do with \tilde{n} , the number of initially identical sub-baths in BH , being sufficiently large, while system S only has one copy of itself.

2.5 Comparisons with quantum imaginary-time evolution (QITE)

Mixing thermal operations seem to relate to the question of quantum imaginary-time evolution (QITE) [13], though this turns out to be partially an illusion. Indeed, if mixing thermal operations are just

examples of QITE, then quantum complexity results in QITE [13] would contradict efficiency of mixing thermal operations in computing ground states.

In QITE, instead of evolving an initial time-zero state over real time duration t under some universe Hamiltonian H , the intention is to evolve the initial state in imaginary time ($t = -i\tau$). Mathematically, $|\psi(\tau)\rangle = e^{-\tau H}|\psi(0)\rangle / \|e^{-\tau H}|\psi(0)\rangle\|$. A key difference is that QITE is pure state evolution: a pure state evolves to a pure state after unit norm normalization by the denominator, even though $e^{-\tau H}$ seems to suggest mixed state evolution. QITE is fundamentally about amplifying or attenuating energy basis amplitude according to $e^{-\tau E}$, where E is energy, and quantum states themselves do not decohere. By contrast in mixing thermal operations, while system outcome probability decays by $e^{-\beta E}$, initially pure system states evolve to mixed states at finite temperature. Considering purity as a quantum resource for further computations, QITE solves more difficult problems but at cost of significant quantum complexity.

An example would be beneficial to demonstrate the key difference. Suppose we initially have some unknown state $|\psi\rangle = a_i|0\rangle + b_i|1\rangle$. We want to amplify amplitude at $|0\rangle$ (considered as energy basis), but it is unclear whether coefficient a_i is non-zero. If $a_i = 0$, then QITE, regardless of Hamiltonians, must preserve $|\psi\rangle \propto |1\rangle$. For mixing thermal operations, the case is different: it does not matter whether a_i is zero or non-zero, since fixed points (equilibrium states) are reached regardless of initial conditions. If baths involved have zero temperature, then ground states of a given Hamiltonian would be reached.

The aforementioned difference is a key reason why CHPZ [7] can attempt to escape the traditional bounds for unstructured quantum search. As with adiabatic quantum computing, the goal is to compute states close to the ground state of a given Hamiltonian. This is not about Grover-style amplitude amplification.

2.6 Comparisons with adiabatic quantum computing and energy gap intuitions

As with adiabatic quantum computing (AQC), mixing thermal operations deal with a system Hamiltonian, and its ground state or states close to it is may be of our interest.

To describe briefly, AQC attempts to compute the ground state of system Hamiltonian H_S by evolving the initial state that is the ground state of some well-understood Hamiltonian H' with the time-varying Hamiltonian. This time-varying Hamiltonian slowly changes from H' to H_S - this process relies on the

well-known adiabatic theorem [9]. Quantum thermal search of this paper (and implicitly, CHPZ [7]) relies on a thermal operation, where the system undergoes open-system evolution. Since the universe still evolves unitarily under time-invariant Hamiltonian, what happens instead, as noted in subsection 2.4, is that initial system state differences are ‘transferred’ to baths in interaction, as the system state converges to the Gibbs state at initial bath temperature.

2.6.1 Energy flow/gap intuitions

Given that mixing thermal operations compute ground states efficiently, we need to consider what may prevent such computations. This could be explained in terms of energy flow and gap.

In mixing thermal operations, energy exchange between system S and bath BH is critical for equilibration at bath temperature. The problem is that BH gets energy inflow, and the equilibration process has diminishing returns (state variations) as time goes on. This issue was tackled by introducing \tilde{n} initially identical sub-baths in bath BH such that each application of mixing thermal operation ϕ utilizes an unused sub-bath. The entire operation then was $\phi^{\tilde{n}}$, and Equation (6) showed that the $\tilde{n} \rightarrow \infty$ limit is largely accurate, which can be treated as the infinite-dimensional or large-bath limit.

This can be alluded to energy gap issues in AQC, where energy gap rapidly diminishes such that exploiting the adiabatic theorem is no longer efficient. With $\tilde{n} = O(1)$, it is possible that similar issues arise - energy flow changes bath BH significantly such that the final equilibrium is at states far away from the ground state.

2.6.2 Limitations of mixing thermal operations

Despite somewhat optimistic results, there is one problem with mixing thermal operations, which is the initial (sub-)bath state. If we want to find the ground state of Hamiltonian H_S , then bath BH ideally has to be at zero temperature, which implies a pure state. But in practice, it is difficult to obtain exact pure states, and some deviations must be expected.

Indeed, this is one practical reason why CHPZ [7] considers bath temperatures that are comfortably non-zero, not vanishingly (negligibly) small. Can we be content with bath states that are not exponentially close to zero-temperature states? Equivalently, in terms of inverse bath temperature, we ask

whether scaling better than polynomial inverse bath temperature scaling ($\beta_{BH} = O(n^k)$, with 2^n being the system Hilbert space dimension) exists. This question is now answered negatively for mixing thermal operations, which is the point to be made in subsection 2.7.

2.7 On polynomial inverse temperature scaling

Let $g(x) : \{0, 1, 2, \dots, 2^n - 1\} \rightarrow \{0, 1\}$ be an unknown function, and let system Hamiltonian H_S be given as follows:

$$H_S = \sum_{x=0}^{2^n-1} g(x) |x\rangle\langle x| \quad (7)$$

We now consider two extreme cases for $g(x)$, re-labelled as $g_0(x)$ and $g_1(x)$:

- $g_0(x)$: every x has $g_0(x) = 1$. H_S for $g_0(x)$ is re-labelled as H_{S,g_0} .
- $g_1(x)$: only one of x satisfies $g_1(x) = 0$, and rest have $g_1(x) = 1$. H_S for $g_1(x)$ is re-labelled as H_{S,g_1} .

Then:

- For H_{S,g_0} , its Gibbs states are the same regardless of temperature, since every energy eigenstate has same energy. Therefore, in the $\tilde{n} \rightarrow \infty$ limit, a composition of \tilde{n} identical mixing thermal operations $\phi^{\tilde{n}}$ results in the unique Gibbs state ρ_m :

$$\rho_m \equiv \frac{1}{2^n} \sum_{x=0}^{2^n-1} |x\rangle\langle x| \quad (8)$$

In this case, any bath temperature is sufficient to compute a ground state, since ρ_m is a ground state.

- For H_{S,g_1} , under a composition of \tilde{n} identical mixing thermal operations $\phi^{\tilde{n}}$, the final equilibrium depends on the initial bath temperature, since one energy eigenstate $|v\rangle$ has different energy from other eigenstates. We now note that probability for $|v\rangle$ in the final equilibrium, assuming inverse bath temperature β_{BH} goes as:

$$P(|v\rangle) = \frac{1}{(2^n - 1)e^{-\beta_{BH}} + 1} \quad (9)$$

Therefore, if we are to arrive at states reasonably close to the ground state $|v\rangle$, $\beta_{BH} = O(n^k)$: polynomial inverse temperature scaling relative to n . (For example, for $\beta_{BH} = 0$ (infinite bath temperature), the denominator is 2^n , while for $\beta_{BH} = 1$, the denominator is approximately $2^n/e$, which changes $P(|v\rangle)$ very little.)

Thus, polynomial inverse bath temperature scaling is necessary for some Hamiltonians, as exemplified by H_{S,g_1} .

3 Conclusion

Polynomial inverse bath temperature scaling of quantum thermal search (and CHPZ [7]) to obtain states close to the ground state of system Hamiltonian H_S could be somewhat problematic, in sense that it demands exponential precision to the bath state to operate. But once this problem is cleared away, a mixing thermal operation can find the ground state of H_S efficiently, as suggested in [7].

This paper simplified the analysis of [7] with a mixing thermal operation that is commonly used in quantum thermodynamics literature [4, 8, 6, 14]. Instead of looking at the entire evolution trajectory, the focus was on the final equilibrium that the system state converges to. In the large-bath (infinite-dimensional) limit ($\tilde{n} \rightarrow \infty$ limit), the final system equilibrium is the Gibbs state at initial bath temperature. Additionally, Equation (6) shows that due to exponential error decay in \tilde{n} , large but non-exponential \tilde{n} is sufficient in order for the infinite-dimensional limit to be valid.

Therefore, as long as bath BH is close to zero temperature, system S cools to the ground state under mixing thermal operations in the large- \tilde{n} limit. Initial system state differences are washed away to bath BH , implying that the final bath equilibrium state is not necessarily a Gibbs state - this explains why there is no violation of the BBBV theorem, despite the universe evolving unitarily.

We conclude with a remark about state purification that was not fully explored in this paper. Suppose system S and bath BH are both initially in pure states, and BH is initially in the ground state in bath Hamiltonian H_{BH} . In the large- \tilde{n} limit, universe Hamiltonian H for mixing thermal operations $\phi^{\tilde{n}}$ first evolves both subsystems into mixed states and then put them back into states close to pure ones at some time t . This may remind us of black hole evaporation [12, 16]: consider S as the black hole exterior and BH as the black hole interior. S interacts with pure states in BH , intermediately resulting in highly

mixed states - but at the end, both S and BH purify. That is, despite the conventional misunderstanding that thermal interactions must always increase system entropy, it can decrease without sacrificing unitary evolution of the universe. Tracing out BH at the end of the interaction (or ‘end of evaporation’), what we have is the equilibrium state of S that is a pure state and also the ground state - initial system state information is lost, transferred away to BH . Initial pure state to final pure state evolution of system S is preserved, but with effective information loss, since initial system information is now in BH which can no longer be accessed after complete evaporation of BH .

The idea of using multiple black hole copies in black hole physics is not unheard of, as can be noticed in (though not restricted to) the recent replica wormhole proposal [2, 15] - indeed, the name ‘replica’ comes from multiple copies of an identical black hole, with replica-related corrections to entanglement entropy of BH in Euclidean path integrals (though replica wormholes take the $\tilde{n} \rightarrow 1$ limit at the end to obtain entanglement entropy). Most simply (without referencing replica wormholes), we could just assume that the initial state of a black hole is in a product of the black hole ground state and apply mixing thermal operations. This should be of significant interests, especially given that CHPZ authors also are heavily involved in computational aspects of black hole physics - sufficiently many copies of BH and mixing thermal operations are sufficient to restore unitary evolution of system (or black hole exterior) S . The exact nature of this coincidence is left to future works.

Declaration of interests

The author(s) have no funding source to declare. Furthermore, there is no conflict of interests.

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