Dissipative search of an unstructured database

Armen E. Allahverdyan [1] and David Petrosyan [1,2]

[1]*A. Alikhanyan National Science Laboratory (YerPhI), 0036 Yerevan, Armenia*
[2]*Institute of Electronic Structure and Laser, FORTH, GR-70013 Heraklion, Crete, Greece*

The search of an unstructured database amounts to finding one element having a certain property out of N elements. The classical search with an oracle checking one element at a time requires on average $N/2$ steps. The Grover algorithm for the quantum search and its unitary Hamiltonian evolution analog accomplish the search asymptotically optimally in $O(\sqrt{N})$ time steps. We reformulate the search problem as a dissipative, incoherent Markov process acting on an N-level system weakly coupled to a thermal bath. Assuming that the energy levels of the system represent the database elements, we show that, with a proper choice of the spectrum and long-range but bounded transition rates between the energy levels, the system relaxes to the ground state, corresponding to the sought element, in time $O(\ln N)$.

I. INTRODUCTION

In a classical search of an unstructured set of N elements, finding an element with a specific feature—verified by some function (oracle) applied to each element at a time—involves on average $N/2$ steps [1]. One of the hallmarks of quantum computation is the Grover search algorithm, which yields quadratic speedup of the search time $\tau = O(\sqrt{N})$ [2,3]. The quantum search can be formulated as a Hamiltonian evolution of an analog quantum system [4]. The N elements of the set are associated with the orthonormal basis states $\{|w_k\rangle\}_{k=1}^N$, one state $|w_\ell\rangle$ corresponding to the sought element having the energy $\epsilon \neq 0$, while the energies of all the other states $|w_{k\neq\ell}\rangle$ are zero. The Hamiltonian of the system is then

$$H_0 = \epsilon |w_\ell\rangle \langle w_\ell|, \tag{1}$$

where ϵ is a known constant, but ℓ is not known. To find ℓ, and thereby $|w_\ell\rangle$, one prepares the system in the equally weighted superposition state $|\psi(0)\rangle = |s\rangle \equiv \frac{1}{\sqrt{N}} \sum_{k=1}^N |w_k\rangle$ [5] and adds to H_0 the interaction Hamiltonian $V = \epsilon |s\rangle \langle s|$ that couples all the basis states,

$$\langle w_l|V|w_k\rangle = \frac{\epsilon}{N} \quad \forall l, k. \tag{2}$$

The system evolution is governed by the Schrödinger equation, and at time $\tau = \frac{\pi \hbar}{2|\epsilon|} \sqrt{N}$ the system attains the desired state $|\psi(\tau)\rangle = |w_\ell\rangle$ [4]. The time τ does not depend on ℓ, and the evolution should be terminated immediately thereafter in order for the target state $|w_\ell\rangle$ to be correctly identified. The asymptotic scaling of the search time $\tau = O(\sqrt{N})$ is optimal for the coherent quantum evolution [3], and it can also be deduced from the time-energy uncertainty relation [6] applied to the Hamiltonian $H_0 + V$ acting on $|\psi(0)\rangle$.

Here we demonstrate an exponential speedup of the search by using, instead of the coherent Schrödinger dynamics that generates unitary evolution, a dissipative Markov dynamics with long-range but bounded transition rates between the energy levels. This system differs from the standard quantum computation paradigm in terms of computational resources (see Appendix A 2). We begin again with the Hamiltonian (1), assuming that $\epsilon < 0$ and therefore $|w_\ell\rangle$ is the ground state of H_0. We then add an auxiliary (known) Hamiltonian H_1 which lifts the degeneracy of all the energy levels $|w_k\rangle$, but still leaves $|w_\ell\rangle$ as a ground state of $H = H_0 + H_1$ for any ℓ, with some energy gap Δ_ℓ. We next couple the system to a thermal bath at a temperature $T = 1/\beta$ ($k_B = \hbar = 1$) and let it relax to the Gibbsian (equilibrium) state described by the density operator $\rho \propto e^{-\beta H}$. If T is sufficiently low, such that $\Delta_\ell \beta > 1$ for any $\ell = 1, 2, \ldots, N$, then $\rho \approx |w_\ell\rangle \langle w_\ell|$, and this approximation can be made arbitrarily precise by increasing the energy gap Δ_ℓ or decreasing the temperature T.

The working time of our dissipative analog device τ_{rlx} is proportional to the inverse relaxation rate α^{-1} of the system towards the equilibrium state ρ, and our main goal is to estimate this time, given the spectrum of the system and its coupling to the thermal reservoir, as detailed below. In contrast to the coherent quantum search, however, we need not demand that τ_{rlx} be independent on the unknown index ℓ, because once the system reaches the equilibrium state $\rho \approx |w_\ell\rangle \langle w_\ell|$, it will remain in that state thereafter. We can then take the search time as $\tau_{\text{rlx}} = \max_\ell [1/\alpha(\ell)]$.

II. THE SYSTEM

We now turn to a more quantitative description of the system. The Hamiltonian H_1 that shifts the energy levels $|w_k\rangle$ should leave $|w_\ell\rangle$ as a unique ground state of $H = H_0 + H_1$ for any ℓ. Assuming for simplicity that H_1 commutes with H_0,

we therefore require that spectrum$[H_1] = \{\eta_k\}_{k=1}^N$ satisfies the condition

$$\eta_N - \eta_1 < |\epsilon|, \tag{3}$$

where $\eta_N = \max\{\eta_k\}$ and $\eta_1 = \min\{\eta_k\}$. We thus have spectrum$[H] = \{\varepsilon_k\}_{k=1}^N = \{\epsilon + \eta_\ell, \{\eta_k\}_{k\neq\ell}\}$ with the smallest energy gap between state $|w_\ell\rangle$ and all the other states $|w_k\rangle$ being $\Delta_N = \eta_1 - (\eta_N + \epsilon) > 0$.

The (incoherent) Markov dynamics of the system weakly coupled to a thermal bath is governed by the rate equations for the populations p_k of states $|w_k\rangle$ (see Appendix A):

$$\dot{p}_k = \sum_{l=1}^N v_{kl} p_l - p_k \sum_{l=1}^N v_{lk}, \tag{4}$$

where $v_{kl} \geqslant 0$ ($v_{kk} = 0$) are the transition rates between the energy levels induced by the thermal bath at temperature T. Hence, we have the detailed balance condition

$$v_{kl} e^{-\beta\varepsilon_l} = v_{lk} e^{-\beta\varepsilon_k}, \tag{5}$$

which implies that there is a unique stationary state of the system determined by the Gibbs (equilibrium) probabilities $p_k = Z^{-1} e^{-\beta\varepsilon_k}$ for $k = 1, 2, \ldots, N$, with $Z = \sum_{k=1}^N e^{-\beta\varepsilon_k}$. In view of the spectrum of the Hamiltonian H, the probability of the ground state is

$$p_1^{(\text{eq})} = \left[1 - e^{\beta\epsilon} \left(e^{\beta\eta_\ell} \sum_{k=1}^N e^{-\beta\eta_k} - 1 \right) \right]^{-1}, \tag{6}$$

and $P_{\text{err}} = 1 - p_1^{(\text{eq})}$ is then the error probability of our dissipative search. Obviously, the smallest ground-state probability in the stationary state, and thus the largest error, would occur for $\ell = N$ with the ground state having the largest possible energy $\epsilon + \eta_N$, see Eq. (3). To ensure the ground-state dominance, we therefore require that $e^{\beta|\epsilon|} \gg (e^{\beta\eta_N} \sum_{k=1}^N e^{-\beta\eta_k} - 1)$.

We are interested in the dependence of the relaxation time to the equilibrium state on N. We therefore demand that the total transition rate from any state $|w_k\rangle$ be bounded,

$$\gamma_k \equiv \sum_{l=1}^N v_{lk} \lesssim v \quad \forall k, \tag{7}$$

where v is some constant independent on N [see Eq. (9) below]. This condition determines the physically acceptable transition rates v_{kl} and excludes parallel relaxation processes that would lead to a trivial acceleration of the dynamics.

Condition (7) automatically holds for short-range transitions: $v_{kl} \sim v \neq 0$ only for $|k - l| \leqslant r$ with some fixed range r that does not depend on N. But then, starting from any arbitrary state $|w_k\rangle$, we will reach the desired ground state $|w_\ell\rangle$, where the population accumulates, via diffusive transport, and the relaxation time will scale as $\tau_{\text{rlx}} = O(N^2)$ [7,8]. This is worse than using either ballistic transport or classical search with the $\tau = O(N)$ scaling. We shall therefore consider long-range but bounded (7) transition rates $v_{kl} > 0 \, \forall k \neq l$.

We can rewrite Eq. (4) for the vector $p = [p_1, p_2, \ldots, p_N]^T$ in a matrix form,

$$\dot{p} = A p, \quad A_{kl} \equiv v_{kl} - \delta_{kl}\gamma_k, \tag{8}$$

where $A_{k\neq l} \geqslant 0$ and $\sum_{k=1}^N A_{kl} = 0$. If follows from Eq. (5) that $\tilde{A}_{kl} = A_{kl} e^{-\frac{\beta}{2}(\epsilon_l - \epsilon_k)} = \tilde{A}_{lk}$ is a symmetric matrix that has the same eigenvalues as A_{kl}. Hence the eigenvalues of A are real. Assuming that A is imprimitive, $[A^m]_{k\neq l} > 0$ for a sufficiently large integer m, we can employ the Perron-Frobenius theorem [8–10] to argue that the largest eigenvalue α_1 of A is zero and nondegenerate. Hence, all the other eigenvalues are negative, $\alpha_1 = 0 > \alpha_2 \geqslant \alpha_3, \ldots$. Note that $0 \geqslant \alpha_2 \geqslant \alpha_3, \ldots$ follows directly from the much simpler Gershgorin's circle theorem [10]. The largest nonzero eigenvalue α_2 of A defines the (exponential) relaxation time $\tau_{\text{rlx}} = 1/|\alpha_2|$ of the master equation (8) (see Appendix B).

The detailed balance condition (5) and the requirement that A be imprimitive still leaves some freedom in choosing the transition rates v_{kl}. A well-known phenomenological approach is to use the Glauber rates [11] widely employed in statistical mechanics [12,13]. We thus assume

$$v_{kl} = \frac{v}{\max(n_k, n_l)} (1 + e^{-\beta\varepsilon_l + \beta\varepsilon_k})^{-1}, \tag{9}$$

where v is the bare relaxation rate that depends on the strength of the system-bath coupling, but does not depend on N and on the number of levels n_k with energies not larger than ε_k. The physical meaning of Eq. (9) is that transitions from higher to lower energy levels are facilitated, while the reverse transitions are suppressed, with the condition (5) obviously satisfied. The Glauber rates are usually written without the factor $1/\max(n_k, n_l)$, but since we allow transitions between all energy levels, this factor is needed to satisfy condition (7). The Glauber rates can be deduced from the Born-Markov treatment of weak system-bath coupling with an appropriate bath spectrum (see Appendix A 1).

Consider first the trivial case of $H_1 = 0$, i.e., all states have the same energy equal to zero, and the ground-state energy is $\epsilon < 0$. From Eqs. (4) and (9), we obtain for the ground-state population

$$\dot{p}_1 = \frac{v}{N(1 + e^{\beta\epsilon})} - \frac{p_1}{\tau_{\text{rlx}}}, \quad \frac{1}{\tau_{\text{rlx}}} = \frac{v}{N} \frac{1 + (N-1)e^{\beta\epsilon}}{1 + e^{\beta\epsilon}},$$

which leads to the equilibrium population $p_1^{(\text{eq})} = [1 + (N-1)e^{\beta\epsilon}]^{-1}$ attained exponentially for times $t \gg \tau_{\text{rlx}}$. Thus the ground-state dominance, $p_1^{(\text{eq})} \simeq 1$ for $(N-1)e^{\beta\epsilon} \ll 1$, leads to $\tau_{\text{rlx}} = O(N)$, which is the expected result for the classical search of an unstructured set.

To obtain more interesting results, consider the auxiliary Hamiltonian H_1 with a nondegenerate spectrum

$$\eta_k = a \ln(k), \quad k = 1, \ldots, N, \tag{10}$$

where $a > 0$. Hence, the energies η_k grow only slowly (logarithmically) with index k, which justifies the possibility of long-range coupling between the energy levels. We then set $\epsilon = -b \ln(N)$ with the parameter $b > a$, to satisfy the condition (3). In Appendix C we present explicit expressions for the Glauber rates for the logarithmic spectrum (10) and show that condition (7) also holds. The ground-state dominance, $p_1^{(\text{eq})} \simeq 1$, now requires that $N^{b\beta} \gg (N^{a\beta} \sum_{k=1}^N k^{-a\beta} - 1)$, which for $N \gg 1$ is satisfied if $b\beta > \max[1, a\beta]$; see Eq. (6). Indeed, for $a\beta > 1$ we have $N^{a\beta} \sum_{k=1}^N k^{-a\beta} = O(N^{a\beta})$, while for
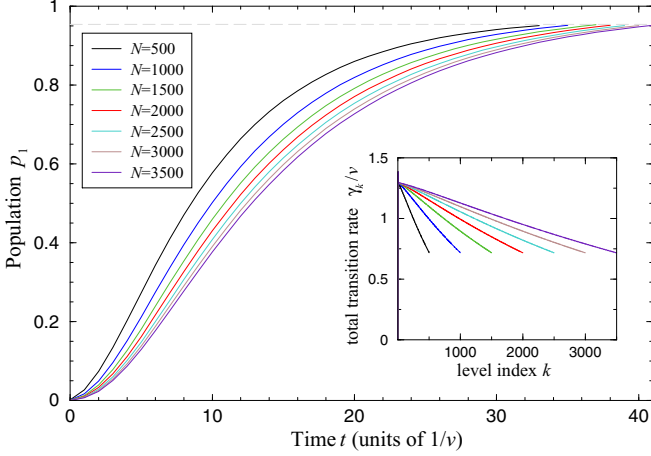
FIG. 1. Dynamics of population of the ground state p_1 (time t is in units of v^{-1}) for various $N = 500, 1000, \ldots, 3500$ (progressively lower curves), as obtained from the numerical solution of Eq. (4) for the system with logarithmic spectrum (10) and the corresponding Glauber rates (9), with the parameters $a\beta = 1.2$ and $b\beta = 2$. The initial populations are $p_k = 1/N \ \forall \ k \in [1, N]$, the sought index is $\ell = N$, i.e., the ground-state energy is $\varepsilon_1 = (a - b) \ln N$, and the dynamics is terminated once $p_1 \geqslant 0.95$. The inset shows the transition rates γ_k of Eq. (7). For each curve, the index k runs from 1 to the corresponding N. Curves from top to bottom in the main figure have the same value of N as curves from left to right in the inset, e.g., the top curve on the main figure and the leftmost curve on the inset refer to $N = 500$.

$a\beta < 1$ we have $N^{a\beta} \sum_{k=1}^{N} k^{-a\beta} = O(N)$. The error probability

$$P_{\text{err}} = 1 - p_1^{(\text{eq})} \simeq N^{-(b-a)\beta} \sum_{k=1}^{N} k^{-a\beta} \qquad (11)$$

can be arbitrarily small, $P_{\text{err}} \approx N^{-(b-a)\beta}$, when $a\beta > 1$.

In Fig. 1 we show the dynamics of population of the ground state p_1, as obtained from numerical solutions of the rate equations (4), with the initial population equally distributed among all the energy levels, while the sought index is $\ell = N$ corresponding to the smallest energy gap $\Delta_N = (b - a) \ln N$. We observe that the time at which the ground-state population exceeds some threshold value, e.g., $p_1 \geqslant 0.95$, grows very slowly with increasing the system size N. In the inset of Fig. 1 we show the total transition rates γ_k from levels k, which remain bounded for any N as per condition (7).

In Fig. 2 we show the relaxation time $\tau_{\text{rlx}} = 1/|\alpha_2|$ as a function of N, obtained from the diagonalization of matrix A in Eq. (8). For $a\beta > 1$, $b > a$ and large $N \gg 1$, the relaxation time grows logarithmically with N:

$$\tau_{\text{rlx}} = O(\ln N). \qquad (12)$$

Note that τ_{rlx} depends only weakly on the sought index ℓ, which determines the energy gap Δ_ℓ but also the spectrum of the excited states and its bandwidth, especially for small ℓ. But once the ground-state dominance condition is satisfied, the relaxation time does not change upon increasing $(b - a)$.

The relaxation time τ_{rlx} increases for smaller values of $a\beta$, since then the transition rates between excited levels tend
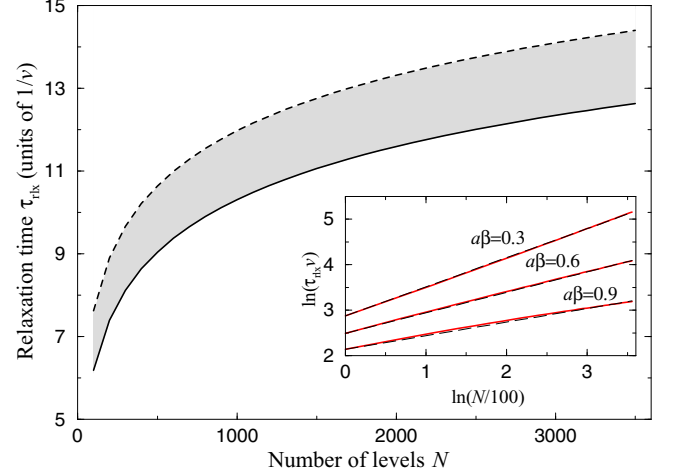

FIG. 2. Relaxation time $\tau_{\text{rlx}} = 1/|\alpha_2|$ (in units of v^{-1}) vs N, as obtained from diagonalization of matrix A in Eq. (8) for the system with logarithmic spectrum (10) and the corresponding Glauber rates (9), with $a\beta = 1.2$ and $b\beta = 2$. For $\ell = N \gg 1$ (solid line) the relaxation time is well approximated by $\tau_{\text{rlx}} v \approx 1.82 \ln N - 2.3$ and for $\ell = 1$ (dashed line) by $\tau_{\text{rlx}} v \approx 1.92 \ln N - 1.34$. Nearly indistinguishable curves are obtained for $(a\beta, b\beta) = (3, 4), (1.2, 4), (1.2, 5)$. The inset shows $\ln(\tau_{\text{rlx}} v)$ vs $\ln(N/100)$ for smaller values of $a\beta$ (red solid lines) and $b\beta = 2$, with each line approximated by $\text{const} + \kappa \ln(N/100)$ (black dashed lines) corresponding to a power-law behavior $\tau_{\text{rlx}} \propto N^\kappa$ with $\kappa = 0.64, 0.45, 0.3$ for $a\beta = 0.3, 0.6, 0.9$, respectively.

to equalize, e.g., for $\ell = N$ we have $v_{kl}/v_{lk} = (l/k)^{a\beta}$ for $l > k > 1$ (see Appendix C). In other words, for smaller $a\beta$, the system wanders longer among the excited levels before relaxing to the ground state.

For $a\beta$ sufficiently smaller than 1, the relaxation time follows a power law [14]

$$\tau_{\text{rlx}} = O(N^\kappa), \qquad (13)$$

with the exponent $\kappa < 1$ that depends on a; see the inset of Fig. 2. For $a \to 0$, we approach $\kappa \to 1$ of the classical search time, while the error probability is $P_{\text{err}} \sim N^{-(b-1)\beta}$. The transition from the logarithmic (12) to the power-law (13) dependence of τ_{rlx} on N is gradual taking place in the vicinity of $a\beta \simeq 1$. We emphasize that $\kappa < 0.5$, as shown in the inset of Fig. 2, already signifies better scaling of the dissipative search time with N than that of the unitary (Grover) search.

III. CONCLUSIONS

To summarize, we have shown that a dissipative Markov dynamics in a system with a weakly nondegenerate spectrum of $N \gg 1$ states can result in the relaxation of the system to the (unknown) ground state during time $\tau_{\text{rlx}} = O(\ln N)$. The system can be viewed as an analog of an unstructured database of N elements, for which the classical search time scales as $O(N)$ while the optimal quantum search time scales as $O(\sqrt{N})$. We can identify the relaxation time of our system with the search time that has exponentially better scaling with the system size N than either the classical or the fully quantum search.

The necessary condition for achieving the short relaxation times of the system, apart from the (weakly) nondegenerate spectrum, is that the Markov process involves transitions between arbitrary energy levels. We should ensure, however, that these long-range interactions are bounded for any N, since otherwise decreasing the search time with increasing N would be trivial. Note that long-range coupling between energy levels (2) is also present in the Hamiltonian analog of quantum search [4].

Since the Markov dynamics of Eqs. (4) is described in terms of classical probabilities, it is natural to ask whether the considered dissipative search can be implemented on a classical computer using, e.g., Monte Carlo simulations to reach the equilibrium state dominated by the ground state. It can of course be done, but will require a large amount of calculations and computer memory. Indeed, the $N = 2^n$ energy levels may correspond to different configurations of n bits or spins $\{\sigma_i = \pm 1\}_{i=1}^n$. Recall that the energy levels in our dissipative analog device should be (weakly) nondegenerate, which means that we need to realize a weakly interacting n-spin system. We will then have to calculate $\sim N$ different energies for 2^n different configurations and store them in the memory, in order to determine the transition probabilities between the different energy levels. These transitions may involve up to n simultaneous spin-flips ($\sigma_i \to -\sigma_i$). In contrast, in the usual Monte Carlo simulations only one spin is flipped at a time, and the energy difference between the old and new configurations is easy to calculate at each time step.

In our study, we assumed weak system-bath coupling and employed the Glauber rates [11–13] for the transitions between the energy levels. But our results equally hold for other similar coupling schemes, e.g., Arrhenius rates often employed in chemical physics [8,14]. We note that master equations with long-range transition rates are frequently employed for describing glassy systems and amorphous materials [14,15]. Such models often produce results that agree with the experiments, but the relaxation times scale polynomially with N. A proof of principle demonstration of dissipative search can be realized with multilevel molecular systems with incoherently coupled subset of rovibrational levels [16] or with atomic Rydberg systems [17] with a properly tailored broadband (microwave) field that induces transitions between a number of Rydberg energy levels, with rates that mimic those in Eq. (9). Finally, our results may have important and interesting implications for protein folding and similar problems, where macromolecules attain the target (minimal energy) conformations very fast, despite the available huge energy landscape [18,19].

APPENDIX A: DERIVATION OF THE MARKOVIAN MASTER EQUATION FOR A SYSTEM WEAKLY COUPLED TO A THERMAL BATH

We consider a system with Hamiltonian H_S, a thermal bath with Hamiltonian H_B, and their interaction described by Hamiltonian V_I. We assume that the initial state of the system $\rho_S(0)$ is diagonal in the energy representation, and we are interested only in the dynamics of populations of its energy eigenstates $\{|\varepsilon_k\rangle\}$. We further assume that the bath is initially in the thermal equilibrium (Gibbsian) state $\rho_B(0) = \frac{1}{Z} e^{-\beta H_B}$, $Z = \text{tr}[e^{-\beta H_B}]$, at inverse temperature $\beta = 1/T$, and we set for brevity $k_B = \hbar = 1$. The system and the bath are initially uncorrelated, and their combined state is

$$\rho_{SB}(0) = \rho_S(0) \otimes \rho_B(0). \tag{A1}$$

We can represent the time evolution generated by the Hamiltonian of the composite system $H = H_S + H_B + V_I$ as

$$e^{-itH} = \mathcal{T}^* e^{-i \int_0^t dt' \tilde{V}_I(-t')} e^{-it(H_S+H_B)}, \tag{A2a}$$

$$\tilde{V}_I(-t') \equiv e^{-it'(H_S+H_B)} V_I e^{it'(H_S+H_B)}, \tag{A2b}$$

$$U_t \equiv \mathcal{T}^* e^{-i \int_0^t dt' \tilde{V}_I(-t')}, \tag{A2c}$$

where $\mathcal{T}^*$ denotes the time antiordering.

Given the eigenresolution of the system Hamiltonian $H_S = \sum_{k=1}^N \varepsilon_k |\varepsilon_k\rangle\langle\varepsilon_k|$ with $\langle\varepsilon_k|\varepsilon_l\rangle = \delta_{kl}$, and using the assumed commutative initial states

$$[H_S, \rho_S] = 0, \quad [H_B, \rho_B] = 0, \tag{A3}$$

we deduce from $\rho_{SB}(t) = e^{-itH} \rho_{SB}(0) e^{itH}$ that

$$p_k(t) \equiv \langle\varepsilon_k|\rho_S(t)|\varepsilon_k\rangle = \sum_{l=1}^N Q_{kl}(t) p_l(0), \tag{A4}$$

where

$$Q_{kl}(t) = \langle\varepsilon_k|\text{tr}_B[U_t|\varepsilon_l\rangle\langle\varepsilon_l| \otimes \rho_B(0)U_t^\dagger]|\varepsilon_k\rangle \tag{A5}$$

is a stochastic, i.e., probability, matrix: $Q_{kl}(t) \geqslant 0$ and $\sum_{k=1}^N Q_{kl}(t) = 1$. Hence, Eqs. (A4) and (A5) describes a classical (though generally non-Markovian) process.

Note that during the evolution the nondiagonal components (coherences) of the system density matrix $\langle\varepsilon_k|\rho_S(t)|\varepsilon_l\rangle$ may in general be nonzero, even though they were assumed $\langle\varepsilon_k|\rho_S(0)|\varepsilon_l\rangle = 0$ ($k \neq l$) for $t = 0$. Yet the coherences $\langle\varepsilon_k|\rho_S(t)|\varepsilon_l\rangle$ do not explicitly enter Eq. (A4) [their contribution is contained in $Q_{kl}(t)$]. We therefore need not invoke the rotating-wave approximation [20–22], which would be inapplicable for a system having many densely spaced energy levels.

To make the Markov approximation for the transition probabilities $Q_{kl}(t)$, we first expand U_t in Eq. (A2c) to second order in $\tilde{V}_I$:

$$U_t = 1 - i \int_0^t dt' \tilde{V}_I(-t') - \int_0^t dt_1 \int_0^{t_1} dt_2 \tilde{V}_I(-t_2)\tilde{V}_I(-t_1). \tag{A6}$$

We now consider the interaction Hamiltonian

$$V_I = g S \otimes B, \tag{A7}$$

with a weak coupling g between the system S and bath B operators, and assume $\mathrm{tr}_B[B\,\rho_B(0)] = 0$. We then obtain

$$Q_{kl}(t) = \delta_{kl} + q_{kl}(t), \tag{A8}$$

$$q_{kl}(t) \equiv -g^2 \delta_{kl} \int_0^t dt_1 \int_0^{t_1} dt_2 [\langle \varepsilon_k | S(-t_2) S(-t_1) | \varepsilon_k \rangle K(t_1 - t_2) + \langle \varepsilon_k | S(-t_1) S(-t_2) | \varepsilon_k \rangle K(t_2 - t_1)]$$

$$+ g^2 \int_0^t \int_0^t dt_1 \, dt_2 \, \langle \varepsilon_k | S(-t_1) | \varepsilon_l \rangle \langle \varepsilon_l | S(-t_2) | \varepsilon_k \rangle K(t_1 - t_2), \tag{A9}$$

where for the bath correlation function $K(t)$ we used its stationary property $K(t - t') = \mathrm{tr}_B[B(t) B(t') \rho_B(0)] = K^*(t' - t)$. We can collect back the matrix exponent writing Eq. (A8) as

$$Q(t) = e^{q(t)}. \tag{A10}$$

We then calculate

$$\dot{q}_{kl}(t) = -\delta_{kl} g^2 \sum_{m=1}^N [\langle \varepsilon_k | S | \varepsilon_m \rangle \langle \varepsilon_m | S | \varepsilon_k \rangle \kappa_{km}^{(+)} + \langle \varepsilon_k | S | \varepsilon_m \rangle \langle \varepsilon_m | S | \varepsilon_k \rangle \kappa_{mk}^{(-)}]$$

$$+ g^2 [\langle \varepsilon_k | S | \varepsilon_l \rangle \langle \varepsilon_l | S | \varepsilon_k \rangle \kappa_{kl}^{(-)} + \langle \varepsilon_k | S | \varepsilon_l \rangle \langle \varepsilon_l | S | \varepsilon_k \rangle \kappa_{lk}^{(+)}], \tag{A11}$$

$$\kappa_{kl}^{(\pm)} = \int_0^t dt' \, e^{it'(\varepsilon_k - \varepsilon_l)} K(\pm t'). \tag{A12}$$

We next assume that the bath correlations $K(t)$ decay with time t sufficiently quickly. Indeed, the characteristic time $\hbar/(k_B T)$ for $K(t)$ can be much smaller than the time $\tau_{\rm rlx}$ over which the populations p_k change significantly (see below). This is due to that $\tau_{\rm rlx}$ contains a large prefactor g^{-2} and, in general, increases with the number of states N. Hence, we can make the Markov approximation by extending in Eq. (A12) the limit of integration $t \to \infty$,

$$\kappa_{kl}^{(\pm)} \approx \int_0^\infty dt' \, e^{it'(\varepsilon_k - \varepsilon_l)} K(\pm t'). \tag{A13}$$

This means that in Eq. (A10) $q(t)$ is approximately a linear function of time t. Eventually, in the considered Markov limit Eqs. (A4) and (A5) are reduced to the master equation

$$\dot{p}_k = \sum_{l=1}^N v_{kl} p_l - p_k \sum_{l=1}^N v_{lk}, \tag{A14}$$

$$v_{kl} = g^2 |\langle \varepsilon_k | S | \varepsilon_l \rangle|^2 \kappa_{kl}, \tag{A15}$$

$$\kappa_{kl} = \int dt' \, K(t') e^{-it'(\varepsilon_k - \varepsilon_l)}. \tag{A16}$$

Hence, the transition rates v_{kl} are proportional to a symmetric (over k and l) factor $|\langle \varepsilon_k | S | \varepsilon_l \rangle|^2$ multiplied by κ_{kl} that depends only on the energy difference $\varepsilon_k - \varepsilon_l$. In the main text, we employ, at a phenomenological level, the master equation (4) of the same form.

Introducing the eigenresolution for the bath Hamiltonian, $H_B = \sum_i E_i \mathcal{P}_i$, where $\mathcal{P}_i$ are eigenprojectors, $\mathcal{P}_i \mathcal{P}_j = \delta_{ij}$ and $\sum_i \mathcal{P}_i = \hat{1}$, we find from Eq. (A16) that

$$\kappa_{kl} = \frac{1}{Z} \sum_{ij} \mathrm{tr}_B(\mathcal{P}_i B \mathcal{P}_j B \mathcal{P}_i) \, e^{-\beta E_i} \delta[E_i - E_j - (\varepsilon_k - \varepsilon_l)], \tag{A17}$$

which clearly shows that $\kappa_{kl} \geqslant 0$ and satisfies the detailed balance condition of Eq. (5):

$$\kappa_{kl} = \kappa_{lk} e^{\beta(\varepsilon_l - \varepsilon_k)}. \tag{A18}$$

We note that Eqs. (A17) and (A18) can also be derived from the Bochner's theorem and Kubo-Martin-Schwinger conditions [21].

1. Glauber rates

In the main text, we use the Glauber transition rates [see Eq. (9)]

$$v_{kl} \propto (1 + e^{-\beta \varepsilon_l + \beta \varepsilon_k})^{-1}. \tag{A19}$$

Assuming that in Eq. (A15) $|\langle \varepsilon_k | S | \varepsilon_l \rangle|^2$ only weakly depend on the level indexes k, l, we can use Eq. (A16) to determine the necessary form of the bath correlator to obtain the Glauber rates,

$$K(t) = \int \frac{d\omega}{2\pi} \frac{e^{-i\omega t}}{1 + e^{-\omega/T}}$$

$$= \int \frac{d\omega}{2\pi} \frac{e^{-i\omega(t - i\zeta)}}{1 + e^{-\omega/T}} = \frac{T}{2i} \frac{1}{\sinh(\pi t T - i\zeta)}$$

$$= \frac{1}{2}\delta(t) + \frac{T}{2i} \mathcal{P} \frac{1}{\sinh(\pi t T)}, \tag{A20}$$

where on the second line $\zeta \to +0$ serves to regularize the integral for $t \to 0$, and we employed the Sokhotski-Plemelj formula with $\mathcal{P}$ denoting the principal value. Equation (A20) shows that the real part of the bath correlator $K(t)$ relaxes very quickly (i.e., during time $t \sim \zeta \to 0$), while the imaginary part relaxes with a characteristic time $\hbar/(k_B T)$; see [13] for further details on the microscopic realization of the Glauber transition rates.

The quantity ζ^{-1} corresponds to the bandwidth (or the cutoff frequency) of the bath spectrum, which is normally large in

the thermodynamic limit [21]. In particular, it should be much larger than the energy differences of the levels of the system coupled to the bath. In the main text, we employ a logarithmic spectrum of the system with the largest energy difference being proportional to $a \ln(N)$. We then get from $a\zeta \ln(N) \ll 1$ the following limitation on the number of energy level N:

$$N \ll e^{1/(a\zeta)}. \tag{A21}$$

Given a sufficiently small value of $a\zeta$, there is large room for satisfying (A21). This is the advantage of using the logarithmic spectrum.

2. Stinespring theorem

Given nontrivial conditions needed to derive a dissipative Markovian dynamics from the weak-coupling system-bath approach, one may want to compare the dissipative dynamics of a system with a global unitary evolution. To this end, we recall the Stinespring theorem [21,23]: dissipative dynamics that operate on diagonal density matrices correspond to a completely positive map (CPM). Any CPM on an N-dimensional Hilbert space $\mathcal{H}_N$ can be represented as a partial trace of a unitary operator U acting on an N^3-dimensional Hilbert space $\mathcal{H}_{N^3} = \mathcal{H}_N \otimes \mathcal{H}_{N^2}$.

The Stinespring theorem provides a finite-dimensional environment for unitary modeling of a CPM. This conforms to the standard set-up of quantum computation [23] and contrasts with the system-bath approach that generally involves infinite-dimensional (due to the thermodynamic limit) bath models.

The Stinespring theorem, however, cannot be applied to our dissipative search procedure to compare its complexity to that of the unitary Grover search. Indeed, if a unitary evolution U is to be related to the search problem, the Hamiltonian H_{Stin} that generates U in $\mathcal{H}_{N^3}$ should be of form $H_{\text{Stin}} = H_S + H_E + V_I$, where both the environment Hamiltonian H_E living in $\mathcal{H}_{N^2}$ and the interaction Hamiltonian V_I living in $\mathcal{H}_{N^3}$ should not depend on the unknown state $|w_\ell\rangle$ and thereby the Hamiltonian $H_S = H_0 + H_1$ of the system. Otherwise, if the system Hamiltonian, and thereby its ground state $|w_\ell\rangle$, were known, there is nothing to search, and if a unitary transformation should be designed to rotate the state vector from an initial well-defined state, such as, e.g., $|s\rangle = \frac{1}{\sqrt{N}} \sum_{k=1}^{N} |w_k\rangle$, to the (known) final state $|w_\ell\rangle$, it can be done optimally with a complexity $O(1)$ for any given N. Hence, the problem in applying U is that it is not generated by a legitimate search Hamiltonian.

Another hindrance is that $H_{\text{Stin}}(t)$ is generally not time-independent [24]. Moreover, we cannot implement $H_{\text{Stin}}(t)$ via external sources, because it would have to depend on the unknown state $|w_\ell\rangle$. In contrast, the system-bath approach employs a time-independent Hamiltonian.

Hence, the Stinespring theorem does not allow one to conclude that the dissipative search described by a Markovian dynamics should be computationally less efficient than the unitary Grover search in $\mathcal{H}_N$.

APPENDIX B: FORMAL SOLUTION OF THE MASTER EQUATION

We write the master equation for the vector $|p\rangle$ of populations of states $\{|w_k\rangle\}_{k=1}^{N}$ using the Dirac notation,

$$\partial_t |p\rangle = A |p\rangle, \tag{B1}$$

where the matrix elements $A_{kl} \equiv v_{kl} - \delta_{kl} \sum_{j=1}^{N} v_{jk}$, with $v_{kk} = 0$, satisfy $A_{k \neq l} \geqslant 0$ and $A_{kk} = -\gamma_k < 0$. Note that, due to the detailed balance condition, $\tilde{A}_{kl} = A_{kl} e^{-\frac{\beta}{2}(\epsilon_l - \epsilon_k)} = \tilde{A}_{lk}$ is a symmetric matrix that has the same eigenvalues as A_{kl}. Hence, A_{kl} is a diagonalizable matrix with properly defined (orthonormal) left and right eigenvectors. The right eigenvector $|R_1\rangle$ of A with eigenvalue $\alpha_1 = 0$ coincides with the stationary Gibbsian probability [8]: $\sum_{l=1}^{N} A_{kl} e^{-\beta \epsilon_l} = 0$. The corresponding left eigenvector $\langle L_1|$ has all its components equal to 1, as seen from $\sum_{k=1}^{N} A_{kl} = 0$. Writing the eigenresolution of A as

$$A = \sum_{k=1}^{N} \alpha_k |R_k\rangle \langle L_k|, \quad \langle L_k|R_l\rangle = \delta_{kl}, \tag{B2}$$

$$A |R_k\rangle = \alpha_k |R_k\rangle, \quad \langle L_k| A = \alpha_k \langle L_k|, \tag{B3}$$

where $\{|R_k\rangle\}_{k=1}^{N}$ and $\{\langle L_k|\}_{k=1}^{N}$ are the right and left eigenvectors, we can formally solve Eq. (B1) via $e^{At} = \sum_{k=1}^{N} e^{\alpha_k t} |R_k\rangle \langle L_k|$ with $\alpha_1 = 0 > \alpha_2 \geqslant \alpha_3, \ldots$, leading to [8]

$$|p(t)\rangle = e^{At} |p(0)\rangle$$
$$\simeq |p^{(\text{st})}\rangle + e^{-|\alpha_2|t} \langle L_2|p(0)\rangle |R_2\rangle + O(e^{-|\alpha_3|t}), \tag{B4}$$

where $|p^{(\text{st})}\rangle = Z^{-1} \sum_{k=1}^{N} e^{-\beta \varepsilon_k} |w_k\rangle \langle w_k|$, with $Z = \sum_{k=1}^{N} e^{-\beta \varepsilon_k}$, is the stationary state. We can therefore define the relaxation time as $\tau_{\text{rlx}} = 1/|\alpha_2|$.

Spectral features of Markov matrices are needed in many applications and have been extensively studied; see, e.g., [25].

APPENDIX C: GLAUBER RATES FOR THE LOGARITHMIC SPECTRUM

In the main text, we employ the Glauber rates

$$v_{kl} = \frac{v}{\max(n_k, n_l)} (1 + e^{-\beta \varepsilon_l + \beta \varepsilon_k})^{-1}, \tag{C1}$$

for the transitions between the states with energies ε_k and ε_l, and here we present the corresponding explicit expressions for the logarithmic spectrum $\eta_k = a \ln(k)$ of the auxiliary Hamiltonian H_1. Consider first the case of the ground state of H_0 at $\ell = 1$ with energy $\epsilon = -b \ln(N)$. The energy levels of $H = H_0 + H_1$ are $(\varepsilon_1, \varepsilon_2, \ldots, \varepsilon_N) = (-b \ln N, a \ln 2, \ldots, a \ln N)$, and the transition rates (C1) are

$$v_{1l} = \frac{1}{l(1 + l^{-a\beta} N^{-b\beta})}, \quad l > 1, \tag{C2a}$$

$$v_{l1} = \frac{1}{l(1 + l^{a\beta} N^{b\beta})}, \quad l > 1, \tag{C2b}$$

$$\frac{v_{1l}}{v_{l1}} = l^{a\beta} N^{b\beta}, \quad l > 1, \tag{C2c}$$

$$v_{k<l} = \frac{1}{l[1 + (k/l)^{a\beta}]}, \quad l > 1, \ k > 1, \tag{C2d}$$

$$v_{l>k} = \frac{1}{l[1+(l/k)^{a\beta}]}, \quad l > 1, \ k > 1, \tag{C2e}$$

$$\frac{v_{k<l}}{v_{l>k}} = \left(\frac{k}{l}\right)^{-a\beta}, \quad l > 1, \ k > 1 \tag{C2f}$$

Note that for high temperatures $a\beta < 1$ the transition rate v_{lk} from a state with lower energy ε_k to a state with higher energy ε_l is smaller, but comparable with the reverse transition rate v_{kl}, which leads to longer relaxation times τ_{rlx} as is also confirmed numerically. The total transition rate from state $|w_l\rangle$ is then

$$\gamma_1 = \sum_{s=1}^{N} v_{s1} = \sum_{s=2}^{N} s^{-1}(1 + N^{b\beta} s^{a\beta})^{-1}, \tag{C3a}$$

$$\gamma_l = \sum_{s=1}^{N} v_{sl} = \frac{1}{l}(1 + N^{-b\beta} l^{-a\beta})^{-1} + \frac{1}{l}\sum_{s=2}^{l-1}[1+(s/l)^{a\beta}]^{-1}$$
$$+ \sum_{s=l+1}^{N} s^{-1}[1+(s/l)^{a\beta}]^{-1}, \quad l > 1, \tag{C3b}$$

and $\gamma_l \lesssim 1$ holds for any $a\beta > 0$, as required.

The same conclusions hold for other values of ℓ, e.g., for $\ell = N$ the energy levels are $(\varepsilon_1, \varepsilon_2, \ldots, \varepsilon_N) = [(a - b)\ln N, 0, a\ln 2, \ldots, a\ln(N-1)]$ and the transition rates are

$$v_{1l} = \frac{1}{l[1+(l-1)^{-a\beta} N^{-(b-a)\beta}]}, \quad l > 1, \tag{C4a}$$

$$v_{l1} = \frac{1}{l[1+(l-1)^{a\beta} N^{(b-a)\beta}]}, \quad l > 1, \tag{C4b}$$

$$\frac{v_{1l}}{v_{l1}} = (l-1)^{a\beta} N^{(b-a)\beta}, \quad l > 1, \tag{C4c}$$

$$v_{k<l} = \frac{1}{l\{1+[(k-1)/(l-1)]^{\beta a}\}}, \quad l > 1, \ k > 1, \tag{C4d}$$

$$v_{l>k} = \frac{1}{l\{1+[(l-1)/(k-1)]^{\beta a}\}}, \quad l > 1, \ k > 1, \tag{C4e}$$

$$\frac{v_{k<l}}{v_{l>k}} = \left(\frac{k-1}{l-1}\right)^{-\beta a}, \quad l > 1, \ k > 1, \tag{C4f}$$

and for $\varepsilon_k < \varepsilon_l$ we again have $v_{lk} < v_{kl}$, provided $b > a$ which is always assumed. The total transition rate from any state $|w_l\rangle$ is

$$\gamma_1 = \sum_{s=1}^{N} v_{s1} = \sum_{s=2}^{N} s^{-1}[1 + N^{(b-a)\beta}(s-1)^{a\beta}]^{-1}, \tag{C5a}$$

$$\gamma_l = \sum_{s=1}^{N} v_{sl} = \frac{1}{l}[1 + N^{(a-b)\beta}(l-1)^{-\beta a}]^{-1}$$
$$\times \frac{1}{l}\sum_{s=2}^{l-1}\left[1 + \left(\frac{s-1}{l-1}\right)^{a\beta}\right]^{-1}$$
$$+ \sum_{s=l+1}^{N} \frac{1}{s}\left[1 + \left(\frac{s-1}{l-1}\right)^{a\beta}\right]^{-1}. \tag{C5b}$$

[1] When searching an unordered set of N elements, in the best (worst) case the desired element will be found in the first (Nth) step and all cases are equally probable, leading on average to $(N+1)/2$ steps. But if some order is already present in the set, the classical search can proceed much faster than in $O(N)$ steps. Indeed, assume that the elements are indexed by numbers $i_1, i_2, \ldots, i_N$ ordered as $i_1 \leqslant i_2 \leqslant \cdots \leqslant i_N$. These numbers are not known, apart from i_ℓ for the desired element, but we do not know its position ℓ. Then i_ℓ can be found in $O(\log_2 N)$ steps by dividing the set into two halves, checking an element at the intersection of the two halves, and selecting one of the halves for further interrogation, and so on.

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