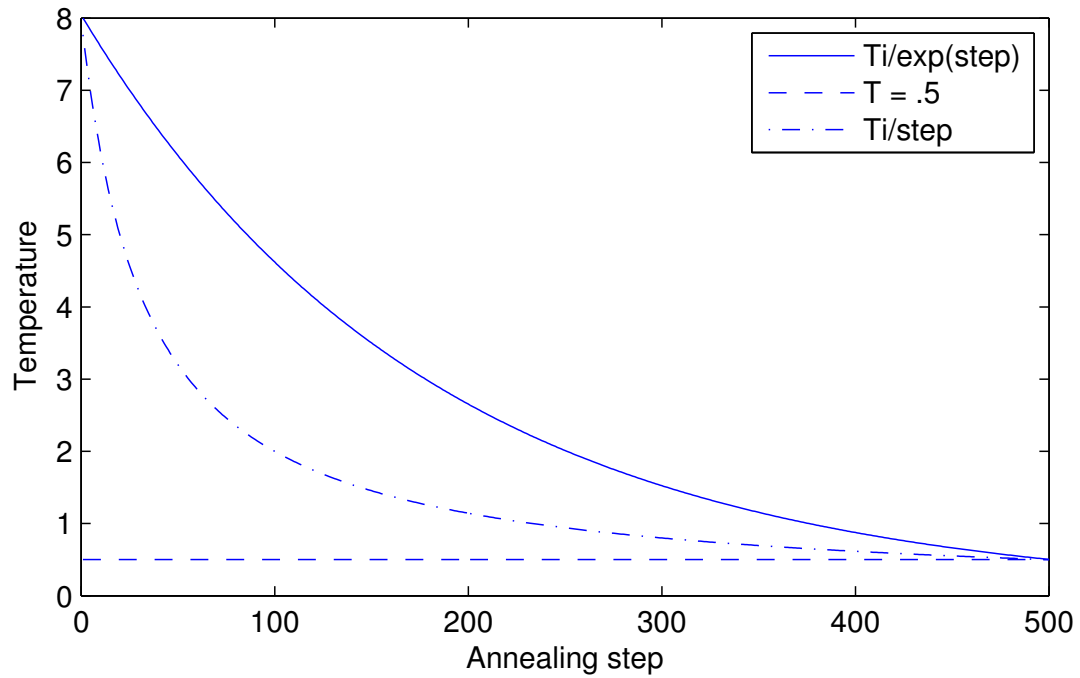
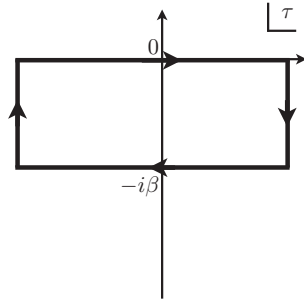


Supplementary Information for “Experimental signature of programmable quantum annealing”

Supplementary Figures



Supplementary Figure S1: **Annealing temperature schedules.** Temperature as a function of annealing step n for three different schedules: exponential $T(n) = T_i r_{\text{exp}}^n$, linear $T(n) = T_i / (nr_{\text{lin}} + 1)$, and constant $T(n) = .5$ temperature, where T_i is the initial temperature, T_f is the final temperature, and $r_{\text{exp}} = (T_f/T_i)^{1/n_{\text{tot}}}$, $r_{\text{lin}} = (T_f/T_i - 1)/n_{\text{tot}}$ for n_{tot} total number of annealing steps.



Supplementary Figure S2: **Contour used in our proof of the KMS condition.**

Supplementary Methods.

First-principles derivation of the master equation

Here we derive the master equation used by SA from first principles within the open quantum systems formalism. This motivates classical SA as a model for a system dominated by classical thermalization of the final Ising Hamiltonian.

Let $H_S(t)$ be the time-dependent system Hamiltonian and $H_{SB} = \sum_{\alpha} A_{\alpha} \otimes B_{\alpha}$ be the system-bath Hamiltonian. We have previously established that the Lindblad equation within the rotating wave approximation has the form¹⁹

$$\begin{aligned} \dot{\rho} = & -i[H_S, \rho] \\ & + \sum_{\alpha\beta} \sum_{\omega} \gamma_{\alpha^*\beta}(\omega) \left[L_{\omega,\beta} \rho L_{\omega,\alpha}^{\dagger} - \frac{1}{2} \{L_{\omega,\alpha}^{\dagger} L_{\omega,\beta}, \rho\} \right], \end{aligned} \quad (\text{S1})$$

where

$$L_{\omega,\alpha} = \sum_{\omega=E_b-E_a} L_{ab,\alpha} = \sum_{\omega=E_b-E_a} |a\rangle\langle a|A_{\alpha}|b\rangle\langle b| \quad (\text{S2a})$$

$$L_{\omega,\alpha}^{\dagger} = \sum_{\omega=E_b-E_a} L_{ab,\alpha}^{\dagger} = \sum_{\omega=E_b-E_a} |b\rangle\langle b|A_{\alpha}^{\dagger}|a\rangle\langle a| \quad (\text{S2b})$$

$\{|a\rangle\}$ is the instantaneous eigenbasis of H_S (we have suppressed its explicit time-dependence) for spin vector $a = \{a_1, \dots, a_N\}$, where $a_i \in \{\uparrow, \downarrow\}$, and

$$\gamma_{\alpha^*\beta}(\omega) = \int_{-\infty}^{\infty} d\tau e^{i\omega\tau} \langle B_{\alpha}^{\dagger}(\tau) B_{\beta}(0) \rangle \quad (\text{S3})$$

is the Fourier transform of the bath correlation function. The star adornment on the first subscript (α^*) is a reminder that the first operator in the bath correlation function is Hermitian-transposed. We have ignored the Lamb shift in Eq. (S1) since for a time-dependent Lindblad evolution it amounts to a small perturbation of the system Hamiltonian. We used this form of the master equation for our quantum open system numerical simulations, as detailed elsewhere¹⁹.

We show below that for a bath in thermal equilibrium at inverse temperature β

$$\gamma_{\alpha^*\beta}(-\omega) = e^{-\beta\omega} \gamma_{\beta\alpha^*}(\omega), \quad (\text{S4})$$

where

$$\gamma_{\beta\alpha^*}(\omega) = \int_{-\infty}^{\infty} d\tau e^{i\omega\tau} \langle B_{\beta}(\tau) B_{\alpha}^{\dagger}(0) \rangle. \quad (\text{S5})$$

We assume that the system-bath coupling Hamiltonian has the form

$$H_{SB} = \sum_{j=1}^N \sum_{r \in \{\pm, z\}} g_j^{(r)} \sigma_j^r \otimes B_j^{(r)}, \quad (\text{S6})$$

where $\sigma^{\pm} = (\sigma^x \pm i\sigma^y)/2$, we identify $|\uparrow\rangle$ with $|0\rangle$ and $|\downarrow\rangle$ with $|1\rangle$, and where we neglect higher-order interactions of the form $\sigma_j^r \otimes \sigma_k^s \otimes B_{jk}^{(rs)}$ or above. Since H_{SB} is Hermitian we also have $B_j^{(\pm)\dagger} = B_j^{(\mp)}$, $B_j^{(z)\dagger} = B_j^{(z)}$, $g_j^{(\pm)*} = g_j^{(\mp)}$, $g_j^{(z)*} = g_j^{(z)}$, and where the asterisk denotes complex conjugation. In the computational basis of spin vectors $\{a\}$, we introduce the notation

$$|a_j^{\pm}\rangle \equiv \sigma_j^{\pm}|a\rangle, \quad (\text{S7})$$

which denotes either a flipping of a_j , or 0 if either σ_j^+ acts on $a_j = \uparrow$ or σ_j^- acts on $a_j = \downarrow$. Then

$$\langle a | \sigma_j^\pm | b \rangle = (\sigma_j^\pm)_{ab} = \delta_{a, b_j^\pm}, \quad (\text{S8})$$

where the δ function is defined to evaluate to zero also when σ_j^\pm annihilates $|b\rangle$. We are interested in classical thermalization, in which the density operator is diagonal in the computational basis $\{a\}$, so we set $\rho_{ab} = 0$ for $a \neq b$. Equation (S1) then gives $\dot{\rho}_{ab} = 0$. Using indexes $\alpha = (r, j)$ and $\beta = (s, k)$ in Eq. (S1), where $r, s \in \{\pm, z\}$ and $j, k \in [1, \dots, N]$, and taking the diagonal $\langle a | \cdot | a \rangle$ matrix element, the Lindblad equation becomes

$$\begin{aligned} \dot{\rho}_{aa} = & \sum_{(r,j), (s,k)} g_j^{(r)*} g_k^{(s)} \times \\ & \sum_{b|b \neq a} \gamma_{(r,j)^*(s,k)}(\omega_{ab}) (\sigma_k^s)_{ab} \rho_{bb} ((\sigma_j^r)^\dagger)_{ba} \\ & - \gamma_{(r,j)^*(s,k)}(\omega_{ba}) ((\sigma_j^r)^\dagger)_{ab} \rho_{aa} (\sigma_k^s)_{ba}, \end{aligned} \quad (\text{S9})$$

where $\omega_{ab} = E_b - E_a$. Note that the sum in Eq. (S1) involving the resonant contribution $\gamma_{\alpha^* \beta}(0)$ from the terms $L_{aa, \beta} \rho L_{bb, \alpha}^\dagger$ and $\frac{1}{2} \{L_{aa, \alpha}^\dagger L_{bb, \beta}, \rho\}$ vanishes since they cancel after taking the diagonal matrix element. Moreover, since Eq. (S9) involves only off-diagonal terms ($b \neq a$), contributions due to σ^z all vanish, and using Eq. (S8), we are left with

$$\begin{aligned} \dot{p}_a = & \sum_{j=1}^N \sum_{r=\pm} |g_j^{(r)}|^2 \left(\gamma_{(r,j)^*(r,j)}(\omega_{aa_j^{-r}}) p_{a_j^{-r}} \right. \\ & \left. - \gamma_{(r,j)^*(r,j)}(\omega_{a_j^r a}) p_a \right), \end{aligned} \quad (\text{S10})$$

where we denoted $p_a \equiv \rho_{aa}$, the probability of spin configuration a . We can furthermore identify

$$P(a \rightarrow a_j^r) \equiv |g_j^{(r)}|^2 \gamma_{(r,j)^*(r,j)}(\omega_{a_j^r a}) \quad (\text{S11a})$$

$$P(a_j^{-r} \rightarrow a) \equiv |g_j^{(r)}|^2 \gamma_{(r,j)^*(r,j)}(\omega_{aa_j^{-r}}) \quad (\text{S11b})$$

as the transition probabilities, so that Eq. (S10) becomes the rate equation

$$\dot{p}_a = \sum_{j=1}^N \sum_{r=\pm} P(a_j^{-r} \rightarrow a) p_{a_j^{-r}} - P(a \rightarrow a_j^r) p_a. \quad (\text{S12})$$

This can be further simplified using the KMS condition. Indeed, note that, using $B_\alpha(\tau) = \sigma_j^\pm(\tau)$ in Eqs. (S3) and (S5), we have

$$\gamma_{(\pm, j)^*(\pm, j)}(\omega) = \gamma_{(\mp, j)(\mp, j)^*}(\omega). \quad (\text{S13})$$

Using this along with $\omega_{a_j^\pm a} = -\omega_{aa_j^\pm}$ and Eq. (S4), we have

$$\gamma_{(\pm, j)^*(\pm, j)}(\omega_{a_j^\pm a}) = e^{-\beta \omega_{aa_j^\pm}} \gamma_{(\mp, j)(\mp, j)^*}(\omega_{aa_j^\pm}). \quad (\text{S14})$$

Therefore Eq. (S11) yields

$$P(a \rightarrow a_j^\pm) = e^{-\beta \omega_{aa_j^\pm}} |g_j^{(\pm)}|^2 \gamma_{(\mp, j)(\mp, j)^*}(\omega_{aa_j^\pm}) \quad (\text{S15a})$$

$$P(a_j^\pm \rightarrow a) = |g_j^{(\mp)}|^2 \gamma_{(\mp, j)(\mp, j)^*}(\omega_{aa_j^\pm}). \quad (\text{S15b})$$

This, together with $g_j^{(\pm)*} = g_j^{(\mp)}$, gives the detailed balance condition for thermalization dynamics

$$\frac{P(a \rightarrow a_j^\pm)}{P(a_j^\pm \rightarrow a)} = e^{-\beta(E_{a_j^\pm} - E_a)} = \frac{f_j(E_a - E_{a_j^\pm})}{f_j(E_{a_j^\pm} - E_a)}, \quad (\text{S16})$$

where we introduced transition functions $f_j(\Delta E)$, which we identify with the transition probabilities in Eq. (S15).

We can now rewrite Eq. (S12) as the classical master equation that we used in our SA numerical simulations

$$\dot{p}_a = \sum_{j=1}^N \sum_{r=\pm} \left(f_j(E_{a_j^r} - E_a) p_{a_j^r} - f_j(E_a - E_{a_j^r}) p_a \right). \quad (\text{S17})$$

Correlation functions and the KMS condition

Here we derive the detailed balance condition Eq. (S4) from first principles. Our calculation closely follows Ref. (19), but differs in that it applies also to non-Hermitian bath operators.

The correlation function of a thermal bath is assumed to satisfy the KMS (Kubo-Martin-Schwinger) condition³⁵

$$\langle B_\alpha^\dagger(\tau) B_\beta(0) \rangle = \langle B_\beta(0) B_\alpha^\dagger(\tau + i\beta) \rangle. \quad (\text{S18})$$

This expression has the advantage that it also applies to operators which are not trace class. For trace class operators the KMS condition can be derived assuming that the bath is in a thermal state, $\rho_B = e^{-\beta H_B}$, where H_B is the bath Hamiltonian. In this case:

$$\begin{aligned} \langle B_\alpha^\dagger(\tau) B_\beta(0) \rangle &= \text{Tr}[\rho_B U_B^\dagger(\tau, 0) B_\alpha^\dagger U_B(\tau, 0) B_\beta] \\ &= \frac{1}{\mathcal{Z}} \text{Tr}[B_\beta e^{-(\beta - i\tau)H_B} B_\alpha^\dagger e^{-i\tau H_B}] \\ &= \frac{1}{\mathcal{Z}} \text{Tr}[B_\beta e^{i(\tau + i\beta)H_B} B_\alpha^\dagger e^{-i(\tau + i\beta)H_B} e^{-\beta H_B}] \\ &= \text{Tr}[\rho_B B_\beta U_B^\dagger(\tau + i\beta, 0) B_\alpha^\dagger U_B(\tau + i\beta, 0)] \\ &= \langle B_\beta(0) B_\alpha^\dagger(\tau + i\beta) \rangle, \end{aligned} \quad (\text{S19})$$

where U_B is the bath unitary evolution operator. Note that

$$\langle B_\alpha^\dagger(\tau) B_\beta(0) \rangle = \langle B_\beta(-\tau - i\beta) B_\alpha^\dagger(0) \rangle. \quad (\text{S20})$$

If in addition the correlation function is analytic in the strip between $\tau = -i\beta$ and $\tau = 0$, then it follows that the Fourier transform of the bath correlation function satisfies the detailed balance condition Eq. (S4) as we show next.

We compute the Fourier transform:

$$\begin{aligned} \gamma_{\alpha^* \beta}(\omega) &= \int_{-\infty}^{\infty} d\tau e^{i\omega\tau} \langle B_\alpha^\dagger(\tau) B_\beta(0) \rangle \\ &= \int_{-\infty}^{\infty} d\tau e^{i\omega\tau} \langle B_\beta(-\tau - i\beta) B_\alpha^\dagger(0) \rangle. \end{aligned} \quad (\text{S21})$$

To perform this integral we replace it with a contour integral in the complex plane, $\oint_C d\tau e^{i\omega\tau} \langle B_\beta(-\tau - i\beta) B_\alpha^\dagger(0) \rangle$, with the contour C as shown in Supplementary Figure S2. This contour integral vanishes by the

Cauchy-Goursat theorem³⁶ since the closed contour encloses no poles (the correlation function $\langle B_\beta(\tau)B_\alpha^\dagger(0) \rangle$ is analytic in the open strip $(0, -i\beta)$ and is continuous at the boundary of the strip³⁷), so that

$$\begin{aligned} \oint_C (\dots) &= 0 \\ &= \int_{\uparrow} (\dots) + \int_{\downarrow} (\dots) + \int_{\rightarrow} (\dots) + \int_{\leftarrow} (\dots) , \end{aligned} \quad (\text{S22})$$

where (\dots) is the integrand of Eq. (S21), and the integral \int_{\rightarrow} is the same as in Eq. (S21). After making the variable transformation $\tau = -x - i\beta$, where x is real, we have

$$\int_{\leftarrow} (\dots) = -e^{\beta\omega} \int_{-\infty}^{\infty} e^{-i\omega x} \langle B_\beta(x)B_\alpha^\dagger(0) \rangle . \quad (\text{S23})$$

Assuming that $\langle B_\alpha(\pm\infty - i\beta)B_\beta(0) \rangle = 0$ (i.e., the correlation function vanishes at infinite time), we further have $\int_{\uparrow} (\dots) = \int_{\downarrow} (\dots) = 0$, and hence we find the result:

$$\begin{aligned} &\int_{-\infty}^{\infty} d\tau e^{i\omega\tau} \langle B_\beta(-\tau - i\beta)B_\alpha^\dagger(0) \rangle \\ &= e^{\beta\omega} \int_{-\infty}^{\infty} e^{-i\omega\tau} \langle B_\beta(\tau)B_\alpha^\dagger(0) \rangle = e^{\beta\omega} \gamma_{\beta\alpha^*}(-\omega) , \end{aligned} \quad (\text{S24})$$

which, together with Eq. (S21), proves Eq. (S4).

Classical master equation explanation for the enhancement of the isolated state

We now explain why, as seen in the numerical simulations shown in the main text, the probability of the isolated state never exceeds that of the average of the 16 cluster ground states, i.e., why

$$p_s \geq \frac{1}{16} \sum_{i=1}^{16} p_i . \quad (\text{S25})$$

Let us first derive a rate equation for the isolated state. A single spin-flip of a core spin in the isolated state raises its energy by 4, since it violates two couplings between the core spins and corresponds to a transition from $|\downarrow\downarrow\rangle$ to $|\uparrow\downarrow\rangle$ (where the second, ancilla, spin is unchanged), which doesn't change the energy according to Eq. (5). Likewise, a single spin-flip of an ancilla spin in the isolated state violates no couplings and corresponds to a transition from $|\downarrow\uparrow\rangle$ to $|\downarrow\downarrow\rangle$ (with the core spin unchanged), which raises the energy by 4 according to Eq. (5). There are 8 ways this can happen (4 core and 4 ancilla spins can be flipped). Since this accounts for all the single spin transitions, Eq. (13) yields the rate equation

$$\dot{p}_s = 8f(-4)p_e - 8f(4)p_s , \quad (\text{S26})$$

where p_e is the population of the excited states with energy -4 . States connected by single spin-flips have similar populations, and all states with energy -4 are connected (see main text). Here we are assuming that the spin flip rate is the same for all sites [corresponding to assuming $g_j^{(r)} = g^{(r)}$ in Eq. (S6)].

We next derive the rate equation for the cluster, once again accounting only for single spin flips. For states in the cluster the core spins are all up, and ancilla-spin flips are energy-preserving transitions between states in the cluster. For core-spin flips we need to analyze two different situations. The first is a configuration in a ground state where the core-ancilla pair starts as $|\uparrow\uparrow\rangle$ and the core spin flips, so the state becomes $|\downarrow\uparrow\rangle$. This violates two couplings, with energy cost 4, and according to Eq. (5) the energy difference between these two states is 4, so the overall result is an excited state with energy 0. The second is a configuration in a ground state where the core-ancilla pair starts as $|\uparrow\downarrow\rangle$ and again the core spin flips, so the state becomes

$|\downarrow\downarrow\rangle$. This again violates two couplings, with energy cost 4, but costs no energy according to Eq. (5), so the overall result is an excited state with energy -4 .

Thus, a state with l ancillae with spin \downarrow and $4-l$ ancillae with spin \uparrow connects (via single spin-flips) to l excited states with energy -4 and $4-l$ excited states with energy 0. To write a rate equation for $p_C = \sum_{i=1}^{16} p_i/16$ we shall assume that all excited states with energy 0 (-4) have probability $p(0)$ (p_e), and all states in the ground state cluster have equal probability p_C . Summing over the number l of ancilla with spin \downarrow for each cluster state, the rate equation is

$$\sum_{i=1}^{16} \dot{p}_i = \sum_{l=0}^4 \binom{4}{l} (lf(-4)p_e - lf(4)p_C) + (4-l)f(-8)p(0) - (4-l)f(8)p_C \quad (\text{S27a})$$

$$= 32(f(-4)p_e - f(4)p_C + f(-8)p(0) - f(8)p_C), \quad (\text{S27b})$$

so that

$$\dot{p}_C = 2(f(-4)p_e - f(4)p_C + f(-8)p(0) - f(8)p_C). \quad (\text{S28})$$

For most temperatures of interest, relative to the energy scale of the Ising Hamiltonian, the dominant transitions are those between the cluster and states with energy -4 . Transitions to energy 0 states are suppressed by the high energy cost, and transitions from energy 0 states to the cluster are suppressed by the low occupancy of the 0 energy states. Then

$$\dot{p}_C \approx 2f(-4)p_e - 2f(4)p_C. \quad (\text{S29})$$

In classical annealing at constant low temperature starting from arbitrary states (that is, the high energy distribution), probability flows approximately $\dot{p}_s/\dot{p}_C \approx 4$ times faster into the isolated state initially, and it gets trapped there by the high energy barrier. This matches well the numerical results of Fig. (3). To show that $p_s \geq p_C$ for slow cooling schedules, assume that this is indeed the case initially. Then, in order for p_C to become larger than p_s , they must first become equal at some inverse annealing temperature β' : $p_s(\beta') = p_C(\beta') \equiv p_g$, and it suffices to check that this implies that p_s grows faster than p_C . Subtracting Eq. (S29) from Eq. (S26) yields

$$\begin{aligned} \dot{p}_s - \dot{p}_C &= 6(f(-4)p_e - f(4)p_g) \\ &= 6f(-4)p_g \left(\frac{p_e}{p_g} - \frac{P(g \rightarrow e)}{P(e \rightarrow g)} \right), \end{aligned} \quad (\text{S30})$$

where in the second line we used Eq. (S16). Now, because the dynamical SA process we are considering proceeds via cooling, the ratio between the non-equilibrium excited state and the ground state probabilities will not be lower than the corresponding thermal equilibrium transition ratio, i.e., $\frac{p_e}{p_g} \geq \frac{P(g \rightarrow e)}{P(e \rightarrow g)} = e^{-4\beta'}$. Therefore, as we set out to show,

$$\dot{p}_s - \dot{p}_C \geq 0, \quad (\text{S31})$$

implying that at all times $p_s \geq p_C$.

The quantum Singular Coupling Limit does not agree with the experimental results Interestingly, an open system QA master equation in the singular coupling limit (SCL) yields results in qualitative agreement with classical thermalization, and opposite to our weak coupling limit (WCL) master equation (S1). Here, following Ref. 36, we present a derivation of the SCL master equation.

We consider a Hamiltonian of the form:

$$H(t) = H_S(t) + \epsilon^{-1}H_I + \epsilon^{-2}H_B, \quad (\text{S32})$$

where we take the interaction Hamiltonian H_I to have the form $A \otimes B$, where the system (A) and bath (B) operators are both Hermitian. The formal solution in the interaction picture generated by H_S and H_B is given by:

$$\tilde{\rho}(t) = \tilde{\rho}(0) - i\epsilon^{-1} \int_0^t ds \left[\tilde{H}_I(s), \tilde{\rho}(s) \right] . \quad (\text{S33})$$

Plugging this solution back into the equation of motion and taking the partial trace over the bath, we obtain:

$$\frac{d}{dt} \tilde{\rho}_S(t) = -\epsilon^{-2} \int_0^t ds \text{Tr}_B \left(\left[\tilde{H}_I(t), \left[\tilde{H}_I(s), \tilde{\rho}(s) \right] \right] \right) , \quad (\text{S34})$$

where we have assumed that $\text{Tr}[\rho_B B] \equiv \langle B \rangle = 0$. Under the standard Markovian assumption that $\rho(t) = \rho_S(t) \otimes \rho_B$ and under a change of coordinates $s = t - \tau$, we can write:

$$\begin{aligned} \frac{d}{dt} \tilde{\rho}_S(t) &= \epsilon^{-2} \int_0^t d\tau \left[(A(t)\tilde{\rho}(t-\tau)A(t-\tau) \right. \\ &\quad \left. - A(t)A(t-\tau)\tilde{\rho}(t-\tau)) \langle B(\tau)B(0) \rangle + \text{h.c.} \right] \end{aligned} \quad (\text{S35})$$

where $A(t) = U_S(t)AU_S^\dagger(t)$ and where we have used the homogeneity of the bath correlation function to shift its time-argument. We change coordinates $\tau = \epsilon^2\tau'$ and observe that under this coordinate change $\langle B(\tau)B(0) \rangle$ is independent of ϵ . We assume that this bath correlation function decays in a time τ_B that is sufficiently fast, such that $\tau_B \ll t/\epsilon^2$. This allows us to approximate the integral by sending the upper limit to infinity. We also assume that $\tau_B \ll \tau'\epsilon^2$, which forces the correlation time of the bath to zero, hence its spectral density to become flat, and hence—using the KMS condition—amounts to taking the infinite temperature limit. Under these assumptions, we can now take the $\epsilon \rightarrow 0$ limit, yielding the SCL master equation

$$\begin{aligned} \frac{d}{dt} \rho_S(t) &= -i [H_S(t) + H_{\text{LS}}, \rho(t)] \\ &\quad + \gamma(0) \left(A\rho(t)A - \frac{1}{2} \{A^2, \rho(t)\} \right) , \end{aligned} \quad (\text{S36})$$

where

$$\gamma(\omega) = \int_{-\infty}^{\infty} d\tau' e^{-i\omega\tau'} \langle B(\tau')B(0) \rangle , \quad (\text{S37})$$

$$H_{\text{LS}} = -A^2 \int_{-\infty}^{\infty} d\omega \gamma(\omega) \mathcal{P} \left(\frac{1}{\omega} \right) , \quad (\text{S38})$$

where H_{LS} is the Lamb shift (renormalization of the system Hamiltonian) and where \mathcal{P} denotes the Cauchy principal value. Thus, even if H_S is time-dependent, we recover the same form for the SCL master equation as in the time-independent case.³⁵

Supplementary References

³⁵ Breuer, H.-P. & Petruccione, F. *The Theory of Open Quantum Systems* (Oxford University Press, 2002).

³⁶ Mathews, J. H. & Howell, R. W. *Complex Analysis: for Mathematics and Engineering* (Jones and Bartlett Pub. Inc., Sudbury, MA, 2012), sixth edn.

³⁷ Haag, R., Hugenholtz, N. M. & Winnink, M. On the equilibrium states in quantum statistical mechanics. *Comm. Math. Phys.* **5**, 215–236 (1967).