Theory of open quantum dynamics with hybrid noise

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Abstract
We develop a theory to describe dynamics of a non-stationary open quantum system interacting with a hybrid environment, which includes high-frequency and low-frequency noise components. One part of the system–bath interaction is treated in a perturbative manner, whereas the other part is considered exactly. This approach allows us to derive a set of master equations where the relaxation rates are expressed as convolutions of the Bloch–Redfield and Marcus formulas. Our theory enables analysis of systems that have extremely small energy gaps in the presence of a realistic environment. As an illustration, we apply the theory to the 16 qubit quantum annealing problem with dangling qubits (Dickson et al 2013 Nat. Commun. 4 1903) and show qualitative agreement with experimental results.

1. Introduction

The theory of open quantum dynamics [1–5] is an important and active area of physics with applications in nanotechnology, chemical physics, quantum biology, and quantum information. In open quantum theories, the system under consideration is assumed to interact with an environment that has many degrees of freedom. Because details of the environmental Hamiltonian are usually unknown, measurable quantities such as temperature $T$ or noise spectrum $S(\omega)$ are used to describe the average statistical behavior of the environment. An open quantum model, therefore, provides a set of differential equations that describe the statistical dynamics of the quantum system, taking the temperature and the spectrum of the bath as input parameters.

Increased research and development of technology in quantum computing and simulation is renewing interest in open quantum modeling. One such promising computation scheme is quantum annealing (QA) [6–8] (in particular, adiabatic quantum computation [9]). In QA, the system is evolved slowly so that it stays at or near the ground state throughout the evolution. At the end of the evolution, the system will occupy a low-energy state of the final Hamiltonian, which may represent a solution to an optimization or a sampling problem. Another important direction of research is related to the simulation of large quantum systems with various quantum hardware [10] including quantum dots [11], ion traps [12, 13], and lattices of coupled superconducting qubits [14, 15].

Open quantum dynamics of a QA processor have been studied theoretically [16–19]. These models assume weak coupling to an environment, which is typically taken to have ohmic spectrum with large high-frequency (HF) content. This limit is well described by the Bloch–Redfield theory [3–5, 17, 20]. Realistic qubits [21], however, suffer from strong interaction with low-frequency (LF) noise (in particular, noise with $1/f$-like spectrum). Incoherent dynamics of a qubit coupled to such an environment are described by the Marcus theory [22–24]. A complete (hybrid) open quantum model should account for both LF and HF environments. Such a model for a single qubit has been developed and agreement with experiment has been demonstrated [25–27]. A generalization of this theory to multiquubit systems has also been developed and compared with experimental observation [28, 29]. Several attempts to combine the Bloch–Redfield and Marcus methods have been undertaken in chemical physics and quantum biology (see, for example, [30–32]).

In this paper, we expand the work of [28, 29]. We provide a systematic and detailed derivation of a hybrid open quantum model, which agrees with the results of [28, 29] for problems with large spectral gaps. Our theory, however, can also be applied to small-gap problems with nonstationary Hamiltonians, for which the model in...
[28, 29] is not applicable. We provide an intuitively appealing and computationally convenient form for the transition rates in terms of a convolution between Redfield and Marcus formulas. As an example, we investigate a dissipative evolution of a 16 qubit system strongly interacting with LF noise and weakly coupled to a HF environment [33]. The problem is characterized by an extremely small gap in the energy spectrum of qubits in the middle of annealing. Solving the problem requires the right combination of Bloch–Redfield and Marcus approaches as well as a proper consideration of the calculation basis, which takes into account the nonstationary effects. The results of the present paper can also be applied to any other open quantum system within the validity range of the approximations.

The paper is organized in the following way. Section 2 describes a single-qubit system to provide the necessary intuition before moving to more complicated multiqubit problems. Section 3 formulates the Hamiltonian and introduces important definitions and notations for the system and the bath. Master equations for the probability distribution of the quantum system are derived in section 4. Section 5 presents the relaxation rates as convolution integrals of the Bloch–Redfield and Marcus envelopes. In the section 6 we show that in equilibrium the master equations obey the detailed balance conditions. We also demonstrate that the convolution expression for the relaxation rates turns into the Marcus or to Bloch–Redfield formulas in the corresponding limits. Dissipative dynamics of a 16 qubit system with an extremely small energy gap is considered in section 7. A brief compilation of the commonly encountered notations is presented in appendix A. In other appendixes we provide a detailed derivation of many important formulas.

2. Single-qubit system

We begin with a single-qubit system interacting with a heat bath. The total Hamiltonian \( H \) of the problem is a sum of three terms:

\[
H = H_S + H_{\text{int}} + H_B,
\]

where \( H_S \) is the Hamiltonian of the single-qubit system, \( H_B \) is the Hamiltonian of the bath, and the Hamiltonian \( H_{\text{int}} \) describes an interaction between the qubit and the bath. The qubit has a Hamiltonian

\[
H_S = -\frac{\Delta}{2}\sigma_x - \frac{\hbar}{2}\sigma_z,
\]

with the Pauli matrices \( \sigma_x, \sigma_y, \sigma_z \), tunneling amplitude \( \Delta \), and bias \( \hbar \). The ground state, \( |1\rangle \), and the excited state, \( |2\rangle \), of the Hamiltonian (2) have energies \( E_{1,2} = \mp \frac{\hbar \Omega}{2} \), with the energy splitting \( \Omega_0 = \sqrt{\Delta^2 + \hbar^2} \). We assume that the free bath (with no coupling to the system) has a Gaussian statistics \([2, 20]\) determined by a spectrum of fluctuations:

\[
S(\omega) = \int dt e^{i\omega t} \langle Q(t) Q(0) \rangle,
\]

where \( Q(t) = e^{iH_B t} Q e^{-iH_B t} \) is a quantum-mechanical operator of the bath. The specific form of the bath Hamiltonian \( H_B \) is not important here, although frequently the Gaussian bath is represented as a collection of quantum harmonic oscillators \([3]\) (see appendix B for more information). The system–bath interaction is commonly determined by the Hamiltonian

\[
H_{\text{int}} = -Q \sigma_z.
\]

In many realistic situations (see, for example, \([27]\)), the noise may come from different sources, some dominating at low frequencies (such as 1/f noise) and others dominating at high frequencies. As such, we consider \( S(\omega) \) to be a sum of two terms:

\[
S(\omega) = S_L(\omega) + S_H(\omega),
\]

where \( S_L(\omega) \) and \( S_H(\omega) \) are functions that are peaked at low and high frequencies, respectively. Each function may tail into the other function’s region. Hereafter we refer to the noise with the spectrum (5) as the hybrid noise. The formula of HF spectrum \( S_H \) is given in section 3.5. For the explicit expression for \( S_L(\omega) \) we refer to equation (B3) shown in the supplementary information section of \([8]\), although there is no need for these formulas here. Notice also that in the present paper we operate with the experimentally-measured parameters of the LF bath, such as the noise intensity \( W^2 \) and the reorganization energy \( \epsilon_L \), which are defined below.

The relaxation dynamics of the qubit become simple in two situations. First, when the qubit is weakly coupled to only a HF bath and the energy splitting of the qubit is larger than the Bloch–Redfield relaxation rate \([3–5]\):

\[
\Gamma = \frac{\Delta^2}{\Delta^2 + \hbar^2} S_H(\Omega_0).
\]

The Bloch–Redfield approach is valid when \( \Gamma \ll \Omega_0 \). Herein, we make the following assumptions for the Boltzmann and Planck constants: \( k_B = 1, \hbar = 1 \).
The second case is when the qubit is coupled only to a LF bath, and its tunneling amplitude $\Delta$ is much smaller than the energy broadening $W$ caused by LF noise: $\Delta \ll W$. The linewidth $W$ and the reorganization energy $\varepsilon_L$ (the shift of the bath energy due to the change of the qubit state) can be found from the formulas

$$W^2 = \int \frac{d\omega}{2\pi} S_L(\omega), \quad \varepsilon_L = \int \frac{d\omega}{2\pi} \frac{S_L(\omega)}{\omega}.$$  \hfill (7)

The qubit dynamics therefore becomes incoherent and the resulting macroscopic resonant tunneling (MRT) rate is given by [25, 26]

$$\Gamma = \frac{\Delta^2}{8} \sqrt{\frac{2\pi}{W^2}} \exp \left\{ -\frac{(h - 4\varepsilon_L)^2}{8W^2} \right\}. \hfill (8)$$

We note that frequency integrals in equations (7) are taken between $-\infty$ and $+\infty$ unless otherwise specified. The reorganization energy $\varepsilon_L$ is defined as a principal value integral. In the case of pure 1/f noise, where $S_L(\omega) \sim \frac{1}{\omega^2}$, the integrals in (7) diverge. To avoid this problem we prefer to use parameters $W$ and $\varepsilon_L$, which are directly extracted from experiments such as performed in [27, 34]. We also note that in the real systems (see, e.g. [35]) the LF spectrum is described as $S_L(\omega) \sim |\omega|^\alpha$ where $\alpha \sim 1$. Even a small deviation of $\alpha$ from one removes divergencies in integrals (7).

The fluctuation-dissipation theorem leads to $W^2 = 2\varepsilon_L T$, where $T$ is the equilibrium temperature of the bath [25]. Equation (8), commonly known as the Marcus formula [22, 23, 30, 31], is valid when the tunneling amplitude $\Delta$ and the rate $\Gamma$ (8) are much smaller than the MRT linewidth $W$: $\Delta \ll W, \Gamma \ll W$. This equation has been successful in explaining experimental data from flux qubits [27, 34].

In practice, low and HF noises coexist and both have to be considered in the dynamics of the qubit. In [25, 27] the formula (8) has been generalized to include effects of HF noise on the MRT rate. For small tunneling amplitudes $\Delta$ the modified rate $\Gamma$ is described by the following integral:

$$\Gamma = \frac{\Delta^2}{4} \int d\tau \ e^{i(h-4\varepsilon_L)\tau - 2W\tau^2} \exp \left\{ 4 \int \frac{d\omega}{2\pi} \frac{S_H(\omega)}{\omega^2} (e^{-i\omega\tau} - 1) \right\}. \hfill (9)$$

We notice that the integrand of equation (9) is equal to the product of the LF component, $e^{-2W\tau^2 - 4\varepsilon_L \tau}$, multiplied by the HF factor, which depends on the spectrum $S_H$. The LF component has the Gaussian Fourier image,

$$G_L(\omega) = \sqrt{\frac{\pi}{2W^2}} \exp \left\{ -\frac{(\omega - 4\varepsilon_L)^2}{8W^2} \right\}. \hfill (10)$$

The HF factor is characterized by the more complicated integral:

$$G_H(\omega) = \int_{-\infty}^{+\infty} d\tau \ e^{i\omega \tau} \exp \left\{ 4 \int \frac{d\Omega}{2\pi} \frac{S_H(\Omega)}{\Omega^2} (e^{-i\Omega \tau} - 1) \right\}. \hfill (11)$$

We notice that both functions, $G_L(\omega)$ and $G_H(\omega)$, satisfy the normalization condition,

$$\int \frac{d\omega}{2\pi} G^\mu(\omega) = 1,$$

where $\mu = L, H$.

The rate (9) can be represented as a convolution of the Gaussian envelope $G_L(\omega)$ and the function $G_H(\omega)$,

$$\Gamma = \frac{\Delta^2}{4} \int \frac{d\omega}{2\pi} G_L(h - \omega) G_H(\omega). \hfill (13)$$

In the Markovian case, where the spectrum $S_H(\omega)$ is flat, $S_H(\omega) = S_H(0)$, the function $G_H(\omega)$ has a Lorentzian shape,

$$G_H(\omega) = \frac{4S_H(0)}{\omega^2 + [2S_H(0)]^2}. \hfill (14)$$

Here we need not to assume that the qubit-bath coupling is small. Equation (14) is valid at frequencies $0 \leq \omega \leq 1/\tau_H$, where $\tau_H$ is a correlation time of the HF fluctuations described by the function $S_H(\omega)$. Later we introduce a spectral density $S_H$ of the ohmic noise characterized by the correlation time $\tau_H \sim 1/T$.

The Bloch–Redfield limit is described by equation (11) with the frequency $\omega$, which is much larger than the coupling to the environment given by the spectrum $S_H(\omega)$: $\frac{S_H(\omega)}{\omega} \ll 1$. With this small parameter, we can expand the dissipative factor in equation (11). Now the function $G_H(\omega)$ turns into the form

$$G_H(\omega) = \frac{4S_H(0)}{\omega^2}. \hfill (15)$$
Equations (14) and (15) can be approximately combined into one Lorentzian formula that has a frequency-dependent numerator,

\[ G^H(\omega) = \frac{4S^H(\omega)}{\omega^2 + [2S^H(0)]^2}. \]  

(16)

The Markovian and Bloch–Redfield expressions follow from this formula in the corresponding limits. Notice also that the function (16) is normalized according to equation (12).

Thus, the single-qubit relaxation rate (9) can be conveniently represented as a convolution of the Gaussian and Lorentzian line shapes,

\[ \Gamma = \Delta^2 \int \frac{d\omega}{2\pi} \frac{S^H(\omega)}{\omega^2 + [2S^H(0)]^2} \sqrt{\frac{\pi}{2W^2}} \exp \left[ -\frac{(h - \omega - 4\varepsilon_L)^2}{8W^2} \right]. \]  

(17)

The convolution integral in (17) has a simple interpretation. One can think of the LF noise as a random shift in energy bias: \( h \rightarrow h + h_{\text{noise}} \), where \( h_{\text{noise}} \) has Gaussian distribution with variance of \( 2W \). The HF relaxation rate, given by the Lorentzian lineshape, will therefore be shifted by \( h_{\text{noise}} \). Ensemble averaging over LF fluctuations will lead to a convolution integral similar to (13) and (17). The reorganization energy \( \varepsilon_L \) is a result of the action of the qubit on the environment. Equation (17) is valid in the limit of small tunneling amplitude \( \Delta \ll W \). In this case the rate \( \Gamma \) is also much less than the MRT line width \( W: \Gamma \ll W \).

It should be mentioned that the intuitive description outlined above holds beyond the validity of equation (17). In the next sections, we will generalize this approach to multiqubit systems without resorting to the small tunneling amplitude approximation.

3. Definitions and notations

3.1. The Hamiltonian

We are interested in dissipative evolution of a quantum annealer [8, 14, 15, 33, 37] treated as a system of \( N \) qubits coupled to a heat bath. The qubits are described by the Hamiltonian:

\[ H_S = \mathcal{A}(s) H_D + \mathcal{B}(s) H_P, \]

(18)

where \( H_D \) and \( H_P \) are the driving (tunneling) and problem Hamiltonians defined as

\[ H_D = -\frac{1}{2} \sum_\alpha \Delta_\alpha \sigma_\alpha^z, \]

\[ H_P = \frac{1}{2} \sum_\alpha h_\alpha \sigma_\alpha^0 + \frac{1}{2} \sum_{\alpha=\beta} J_{\alpha\beta} \sigma_\alpha^+ \sigma_\beta^-. \]

(19)

The energy functions \( \mathcal{A}(s) \) and \( \mathcal{B}(s) \) determine the annealing schedule with \( s = t/t_b \), being the dimensionless annealing parameter \( 0 \leq s \leq 1 \), and \( t \) and \( t_b \) being the running time and the total annealing time, respectively. Details of the annealing schedule are unimportant for the current discussion as long as the time-dependent Hamiltonian changes slowly, which is exactly the case for QA algorithms.

We assume an interaction with a bath of the form:

\[ H_{\text{int}} = -\sum_{\alpha=1}^N Q_\alpha \sigma_\alpha^z, \]

(20)

with operators \( Q_\alpha \), characterized by Gaussian statistics with zero average values, \( \langle Q_\alpha \rangle = 0 \). We also suppose that different qubits, labeled as \( \alpha \) and \( \beta \), are coupled to statistically independent environments, such that \( \langle Q_\alpha Q_\beta \rangle = 0 \) if \( \alpha \neq \beta \). This has been experimentally confirmed for flux qubits [38].

3.2. Schrödinger picture

The total system–bath Hamiltonian \( H \) written in the Schrödinger representation has the form given by equation (1). Here, the time evolution of the system–bath can be described by the density matrix \( \rho_{SB} = |\psi_{SB}\rangle \langle \psi_{SB}| \), where \( |\psi_{SB}\rangle \) is the system–bath wave function. The time-evolution of \( \rho_{SB} \) is governed by the von Neumann equation,

\[ i\dot{\rho}_{SB} = [H_S + H_B + H_{\text{int}}, \rho_{SB}], \]

(21)

where \([A, B]\) means a commutator of operators \( A \) and \( B \). We assume that the initial system–bath matrix can be factorized into the product

\[ \rho_{SB} = \rho_S \rho_B, \]

(22)

where \( \rho_S \) and \( \rho_B \) are the reduced density matrices of the system and bath, respectively. However, in Section 3.3 we will derive an expression for \( \langle Q_\alpha \rangle \) directly from the master equation, which is more convenient for practical applications.

3 Similar convolution form of low- and high-frequency environment factors has been used in [36] for the specific case of a tunneling rate of Cooper pairs in a small Josephson junction.
Here, Tr\(_B\) denotes a trace over bath variables, and \(T\) is the bath temperature. With the unitary matrix \(U_B = e^{iH_B t}\), the Hamiltonian \(H(1)\) turns into the form

\[
H' = U_B^\dagger (H_S + H_{\text{int}} + H_B) U_B - i U_B^\dagger \frac{\partial}{\partial t} U_B
\]

where \(Q_\alpha(t)\) is the free-evolving bath operator,

\[
Q_\alpha(t) = e^{iH_B t} Q_\alpha e^{-iH_B t}.
\]

The evolution of the density matrix can now be defined in terms of the unitary operator

\[
U(t) = T e^{-i \int_0^t \text{d} \tau \dot{H}(\tau)}.
\]

Hereafter, for simplicity of notation, we remove time dependences from unitary matrices. A consecutive application of the operators \(U_B\) and \(U\) produces the system–bath density matrix \(\rho_{SB}(t)\) at time \(t\),

\[
\rho_{SB}(t) = U_B U^{\dagger} \rho_{SB}(0) U^{\dagger} U_B.
\]

This time-dependent matrix presents the solution of the von Neumann equation (21). The average value of an arbitrary Schrödinger operator \(\mathcal{O}\), which describes a physical variable of the qubits or of the bath, is determined by the density matrix \(\rho_{SB}(t)\) (27) at time \(t\),

\[
\langle \mathcal{O} \rangle_{SB}(t) = \text{Tr} \{ \rho_{SB}(t) \mathcal{O} \} = \text{Tr}_B \sum_k \langle k | U^{\dagger} U_B \mathcal{O} U_B U | k \rangle.
\]

Here the total trace \(\text{Tr}\) includes the trace \(\text{Tr}_B\) over free-bath variables and also the trace \(\text{Tr}_S\),

\[
\text{Tr}_S = \sum_k \langle k | \rangle \langle k |\rangle,
\]

over a full set of qubit states \(\{|k\}\) .

3.3. Heisenberg picture

In the theory of open quantum systems interacting with a heat bath [39] the state of the system can be described by the reduced density matrix, which is obtained by averaging the system–bath matrix \(\rho_{SB}\) over the bath fluctuations. Some information about quantum fluctuations is lost after the averaging. This limits the method to calculations of only the averages and same-time correlation functions. Other properties such as different-time correlations remain beyond the reach of this approach. In the Heisenberg picture, the equations are written in terms of the operators without taking averages. This allows calculations of correlation functions to any order as long as the equations can be solved.

In the Heisenberg representation, the average value of an arbitrary operator \(\mathcal{O}\) in (28) can be written as

\[
\langle \mathcal{O} \rangle_{SB}(t) = \text{Tr} \{ \rho_{SB}(0) \mathcal{O}^H(t) \},
\]

where

\[
\mathcal{O}^H(t) = U^{\dagger} U_B^\dagger \mathcal{O} U_B U
\]

is the Heisenberg operator of the variable \(\mathcal{O}\). The Schrödinger operator \(\mathcal{O}\) may explicitly depend on time. In this case, its partial derivative over time, \(\frac{\partial \mathcal{O}}{\partial t}\), is not equal to zero. It follows from equation (31) that the time evolution of the operator \(\mathcal{O}^H(t)\) is described by the Heisenberg equation

\[
i \frac{d}{dt} \mathcal{O}^H = [\mathcal{O}^H, H^H] + (U_B U)^\dagger \frac{\partial \mathcal{O}}{\partial t} U_B U,
\]

where the total Hamiltonian (1) is written in the Heisenberg picture as

\[
H^H = U^{\dagger} U_B^\dagger H U_B U.
\]

3.4. The bath

We assume that the bath coupled to \(\alpha\)-qubit is described by Gaussian statistics [2, 20]. These statistics are characterized by a correlation function \(K_\alpha(t, t')\)
\[ K_\alpha(t, t') = \langle Q_\alpha(t)Q_\alpha(t') \rangle. \]  

(34)

Here \( Q_\alpha(t) \) is a free-evolving bath operator \( (25) \). The brackets \( \langle \cdots \rangle \) denote the average of \( \mathcal{O} \) over the free-bath fluctuations,

\[ \langle \mathcal{O} \rangle = \text{Tr}[\rho_B \mathcal{O}], \]

(35)

unless otherwise specified. For stationary processes, \( K_\alpha(t, t') \) depends on the time difference, hence allowing the spectral density to be defined as

\[ S_\alpha(\omega) = \int dt e^{i\omega t} K_\alpha(t). \]

(36)

In addition to the correlator \( (34) \), we introduce dissipative functions \( f_\alpha(t) \) and \( g_\alpha(t) \) defined as

\[
\begin{align*}
    f_\alpha(t) &= \int \frac{d\omega}{2\pi} \frac{S_\alpha(\omega)}{\omega} \left( 1 - e^{-i\omega t} \right), \\
    g_\alpha(t) &= -i f_\alpha(t) = \int \frac{d\omega}{2\pi} \frac{S_\alpha(\omega)}{\omega} e^{-i\omega t}. 
\end{align*}
\]

(37)

These definitions can be compared to similar functions introduced by equation \( (3.36) \) in \cite{3}. Notice that \( K_\alpha(t) = f_\alpha(t) \). The total reorganization energy of the bath is defined as

\[ \varepsilon_\alpha = \int \frac{d\omega}{2\pi} \frac{S_\alpha(\omega)}{\omega}. \]

(38)

The response of the bath to an external field is described by the retarded Green function

\[ \varphi_\alpha(t - t') = \langle [iQ_\alpha(t), Q_\alpha(t')] \rangle \theta(t - t'). \]

(39)

The causality is provided by the Heaviside step function \( \theta(t - t') \). The response function \( \varphi_\alpha \) is related to the susceptibility of the bath defined through

\[ \chi_\alpha(\omega) = \int dt e^{i\omega t} \varphi_\alpha(t). \]

(40)

According to the fluctuation-dissipation theorem, in equilibrium \( S_\alpha(\omega) \) is proportional to the imaginary part \( \chi''_\alpha(\omega) \) of the bath susceptibility,

\[ S_\alpha(\omega) = \chi''_\alpha(\omega) \left[ \coth \left( \frac{\omega}{2T} \right) + 1 \right], \]

(41)

where \( T \) is the temperature of the equilibrium bath.

### 3.5. Hybrid noise

Hereafter we assume that the dissipative environments coupled to different qubits, although uncorrelated, have the same spectral density of bath fluctuations: \( S_\alpha(\omega) = S(\omega) \). The same is true of the functions \( f_\alpha(\tau) = f(\tau), g_\alpha(\tau) = g(\tau) \), and \( \chi_\alpha(\omega) = \chi(\omega) \). In the case of hybrid noise, \( S(\omega) \) is given by equation \( (5) \). The dissipative functions \( f \) and \( g \) can be split into low and HF components,

\[ f = f_L + f_H, \quad g = g_L + g_H. \]

(42)

For the LF part of the function \( f \), one can expand \( e^{i\omega \tau} \) in equation \( (37) \), assuming \( \omega \tau \ll 1 \). Keeping up the second order in \( \omega \tau \), we obtain

\[ f_L(\tau) = i \varepsilon_L \tau + \frac{1}{2} W^2 \tau^2, \]

(43)

with \( \varepsilon_L \) and \( W \) defined in equation \( (7) \).

To treat the HF parts, we assume Ohmic noise

\[ S_H(\omega) = -\frac{\eta \omega}{1 - e^{-\omega/\omega_T}} e^{-|\omega|/\omega_T}. \]

(44)

Here \( \eta \) is a small dimensionless coupling constant and \( \omega_T \) is a large cutting frequency of the HF noise. This assumption is justified experimentally \cite{27} and also theoretically \cite{3}. The dissipative functions \( f_H \) and \( g_H \) are calculated in appendix \textit{C}. The total reorganization energy, \( \varepsilon_L \equiv \varepsilon \), is defined by \( (38) \), so that \( \varepsilon = \varepsilon_L + \varepsilon_H \). Here \( \varepsilon_L \) is defined in \( (7) \), and \( \varepsilon_H \) is the HF component of the reorganization energy \( (38) \). For the Ohmic spectrum \( (44) \) of the bath, we have \( \varepsilon_H = \frac{\eta \omega}{2\pi} \).

### 3.6. Selection of the basis

The dynamical equations we aim to derive must be represented in a convenient basis, which we denote by \( \{ | n(t) \rangle \} \). This basis could be the instantaneous eigenstates of the system Hamiltonian or some superpositions of those. The system–bath Hamiltonian \( H' \) in \( (24) \) can be written as

\[
H(t) = \sum_{\alpha = \text{HF}, \text{LF}} H_{\alpha}^{S} + \sum_{\alpha = \text{HF}, \text{LF}} H_{\alpha}^{B} + H_{\alpha}^{SB}.
\]
\[ H' = \sum_n [E_n - Q_n(t)] |n \rangle \langle n| + \sum_{m \neq n} [T_{mn} - Q_{mn}(t)] |m \rangle \langle n|, \]  

(45)

where

\[ E_n = \langle n| H_S |n \rangle, \quad T_{mn} = \langle m| H_S |n \rangle, \]  

(46)

\[ Q_n(t) = \sum_{\alpha=1}^{N} \sigma_n^{\alpha} Q_{\alpha}(t), \]  

(47)

\[ Q_{mn}(t) = \sum_{\alpha=1}^{N} \sigma_{mn}^{\alpha} Q_{\alpha}(t), \]  

(48)

with \( Q_{\alpha}(t) \) defined in (25), and

\[ \sigma_n^{\alpha} = \langle n| \sigma_z^{\alpha} |n \rangle, \quad \sigma_{mn}^{\alpha} = \langle m| \sigma_z^{\alpha} |n \rangle. \]  

(49)

We also introduce the following notations, which we will use later:

\[ a_{mn} = \sum_{\alpha} (\sigma_m^{\alpha} - \sigma_n^{\alpha})^2, \quad b_{mn} = \sum_{\alpha} |\sigma_{mn}^{\alpha}|^2, \]  

(50)

\[ c_{mn} = \sum_{\alpha} \sigma_{mn}^{\alpha} (\sigma_m^{\alpha} - \sigma_n^{\alpha}), \quad d_{mn} = \sum_{\alpha} \sigma_{mn}^{\alpha} (\sigma_m^{\alpha} + \sigma_n^{\alpha}). \]  

(51)

Notice that \( a_{mn} \) gives the Hamming distance between \(|m\rangle\) and \(|n\rangle\), if these states are computation basis states. Parameters \( a_{mn} \) and \( b_{mn} \) are real and positive, and \( c_{mn} = -d_{mn} \).

4. System evolution in the interaction representation

Properties of the system of qubits are determined by the reduced density matrix

\[ \rho_S = \text{Tr}_B \rho_{SB} = \text{Tr}_B [U \rho_{SB} (0) U^\dagger], \]  

(52)

where the system–bath density matrix \( \rho_{SB} \) is given by equation (27). A system–bath average of an arbitrary operator \( \mathcal{O}_S \) of the system is written as

\[ \langle \mathcal{O}_{SB} \rangle_S = \text{Tr}_S [\rho_S(t) \mathcal{O}_S]. \]  

(53)

In the basis introduced in section 3.6, the matrix \( \rho_S \) has the form

\[ \rho_S = \sum_{mn} \rho_{mn} |n \rangle \langle m|, \]  

(54)

with the matrix elements defined as

\[ \rho_{mn} = \langle n| \rho_S |m \rangle. \]  

(55)

Our goal is to derive a set of master equations for the probability distribution of the qubits, \( P_n \), over the states \( \{|n\rangle\} \), where

\[ P_n = \rho_{nn} = \langle n| \rho_S |n \rangle. \]  

(56)

The time evolution of the matrix (50) is determined by the unitary operator \( U \) defined by (26) where the Hamiltonian \( H' \) is given by equation (45). The objective is to go beyond the perturbation theory in the system–bath coupling. This can be done by treating \( Q_{\alpha} \) exactly, but \( Q_{mn} \) perturbatively. The interaction representation is best suited for this goal.

A transition to the interaction picture, although straightforward for time-independent bases, becomes more involved if the basis changes in time. Let us introduce a unitary operator

\[ U_0(t) = \sum_n e^{-i \phi_n(t)} S_n(t) |n \rangle \langle n|, \]  

(57)

where \(|n\rangle\) is a time-dependent basis of the system, and

\[ \phi_n(t) = \int_0^t \text{d} \tau E_n(\tau), \]  

(58)

is written in terms of average energies \( E_n(t) = \langle n(t)| H_S(t) |n(t) \rangle \). We also introduce the S-matrix:

\[ S_n(t) = T \exp \left[ i \sum_{\alpha} \sigma_n^{\alpha}(t) \int_0^t \text{d} \tau_1 Q_{\alpha}(t_1) \right], \]  

(59)

with \( T \) being the time-ordering operator for \( t_1 \). Notice that the time-dependent matrix element \( \sigma_n^{\alpha}(t) \) is taken out of the integral over \( t_1 \). This becomes necessary when we want to express correlation functions in terms of dissipative functions.
The interaction Hamiltonian is given by the expression

\[ H_I = U^0 H^I U_0^I - i U_0^I U^I. \] (58)

This Hamiltonian defines the unitary evolution operator

\[ U_I(t) = T e^{-\int_0^t d\tau H_I(\tau)}. \] (59)

The Hamiltonian \( H_I \) does not contain the nonperturbative diagonal terms \( Q_n \). To calculate the time-derivative \( U^0_0 \) in (58), we need

\[-i\dot{S}_0(t) = Q_0(t) S_0(t) + \sum_{\alpha} \alpha^0_n(t) S_0(t) \int_0^t d\tau \tilde{S}_0^\alpha(t, \tau) Q_\alpha(\tau) \tilde{S}_0(t, \tau), \] (60)

where

\[ \tilde{S}_0(t, \tau) = T \exp \left[ i \sum_{\alpha} \alpha^0_n(t) \int_0^\tau d\tau' Q_\alpha(\tau') \right]. \] (61)

Notice that \( S_0(t) = \tilde{S}_0(t, t) \). In the interaction picture, the system–bath Hamiltonian \( H_I \) (58) takes the form

\[ H_I = i \sum_n |n\rangle \langle n| - \sum_{mn} Q_{mn} |m\rangle \langle n|. \] (62)

The modified bath operator \( \tilde{Q}_{mn} \) has diagonal terms

\[ \tilde{Q}_{mn}(t) = -\sum_{\alpha} \alpha^0_n(t) \int_0^t d\tau \tilde{S}_0^\alpha(t, \tau) Q_\alpha(\tau) \tilde{S}_0(t, \tau), \] (63)

and off-diagonal \((m \neq n)\) terms,

\[ Q_{mn} = e^{i\phi_{mn}(t)} S_{mn}^0(t) [Q_{mn}(t) - T_{mn}] S_0(t). \] (64)

Here

\[ \phi_{mn}(t) = \phi_{m}(t) - \phi_{n}(t) = \int_0^t d\tau' \omega_{mn}(\tau'), \] (65)

is defined in terms of

\[ \omega_{mn}(t) = E_m(t) - E_n(t), \] (66)

and

\[ \alpha^0_n(t) = \sum_{mn} [\sigma^0_{mn} \langle n|m \rangle + \langle n|m\rangle \sigma^0_{mn}]. \] (67)

We also introduce

\[ T_{mn} = T_{mn} - i \langle m|n \rangle, \] (68)

with \( T_{mn} \) defined in (46). When the basis \( \{|n\rangle\} \) is formed by the instantaneous eigenstates of the Hamiltonian \( H_0 \), \( H_0|n\rangle = E_n|n\rangle \), we obtain

\[ \langle m|n \rangle = \frac{1}{t_f} \langle m(s) \frac{dE_{mn}(s)}{ds} n(s) \rangle. \] (69)

Here we assume that the spectrum \( E_{mn} \) is nondegenerate and that \( H_0 \) (18) is characterized by real parameters. In this case we have \( \langle m|n \rangle = 0 \).

In appendix D, we calculate correlation functions \( \tilde{K}_{mn}(t, t') \) of the bath variables (64),

\[ \tilde{K}_{mn}(t, t') = \langle \tilde{Q}_{mn}(t), \tilde{Q}_{mn'}(t') \rangle. \] (70)

We show that the only terms that survive during the annealing run are characterized by the relation

\[ K_{mn}(t, t') = \delta_{mm'} K_{mn}(t, t'), \] (71)

where the function \( K_{mn}(t, t') \) is given by equation (D34). In addition, we demonstrate that, during annealing, correlations between diagonal operators \( \tilde{Q}_{kk} \) (63) and off-diagonal bath variables \( Q_{mn} \) (64) rapidly disappear in time, such that \( \langle \tilde{Q}_{mn}(t), \tilde{Q}_{kn}(t') \rangle \sim 0 \). The same is true for the average values of the operators (64): \( \langle \tilde{Q}_{mn}(t) \rangle \sim 0 \).

### 4.1. Time evolution

The evolution of the matrix \( \rho_S \) is determined by the unitary matrix (26), which can be written as: \( U = U_0^I U_I \), where \( U_0^I \) and \( U_I \) are given by equations (55) and (59). In the interaction picture, we have
\[ \rho_{mn} = e^{i\beta_m} \text{Tr}[\rho_S(0)U_d^n |m\rangle \langle m| U_d^m] = e^{i\beta_m} \text{Tr}[\rho_S(0)U_d^n S_n S_m/n|U_d^m], \]
\[ = e^{i\beta_m} \text{Trs}[\rho_S(0) (U_d^n S_n S_m/n|U_d^m)]. \]  

(72)

Here, we have used (22), (50), (33) and have introduced the interaction picture operator

\[ \Lambda_{mn} = U_d^n |m\rangle \langle n| U_d^m, \]

(73)

which will play an important role in our theory. The bath average \( \langle \ldots \rangle \) is defined in (35). Equation (72) takes a simpler form for the diagonal elements:

\[ P_n = \rho_{nn} = \text{Trs}[\rho_S(0) \langle \Lambda_{nn} \rangle]. \]

(74)

In the following, we consider time evolution of the operators \( \Lambda_{mn} \) instead of working with the elements (72) and (74) of the system density matrix. Working with operators instead of averages allows derivation of more accurate master equations.

Taking the derivative of (73) and using (62), we obtain

\[ i \frac{d}{dt} \Lambda_{mn} = \sum_k (Q_{km}^I \Lambda_{kn} - Q_{nk}^I \Lambda_{mk}), \]

(75)

where

\[ Q_{mn}^I = U_d^n \tilde{Q}_{mn} U_d^m. \]

(76)

Here we use the fact that \( \Lambda_{mn} \) and \( Q_{kl}^d \), taken at the same moment of time \( t \), commute: \( [ \Lambda_{mn}, Q^d_{kl} ] = 0 \), for any set of indexes \( m, n, k, l \). The evolution of the diagonal elements \( \Lambda_{nn} \) is of prime interest since these elements determine the probabilities (74):

\[ i \frac{d}{dt} \Lambda_{nn} = \sum_{m \neq n} (Q_{mn}^I \Lambda_{mn} - Q_{nm}^I \Lambda_{nm}). \]

(77)

Notice that the diagonal elements of the bath, \( Q^I_{nm} \) and \( Q^I_{nm} \), have no influence on the evolution of \( \Lambda_{nn} \).

Averaging over free bath fluctuations leads to

\[ i \frac{d}{dt} \langle \Lambda_{nn} \rangle = \sum_{m \neq n} \langle (Q_{mn}^I \Lambda_{mn}) - (Q_{nm}^I \Lambda_{nm}) \rangle. \]

(78)

This equation is exact and difficult to solve without approximations.

To simplify equation (78), in appendix E we use perturbation expansion assuming that the combined operator \( \tilde{Q}_{mn} \) is small. It does not mean that all system–bath interactions are assumed to be small. A part of these couplings described by the operator \( Q_{kl}(t) \) is treated precisely (see equations (47), (63), (64) for definitions). In appendix E we take into account the above-mentioned perturbative approximation and express the right-hand side of equation (78) in terms of products of bath and system correlation functions, such as \( \tilde{K}_{mn}(t, t') \langle \Lambda_{mn}(t) \Lambda_{nm}(t') \rangle \). In appendix D we find that the bath correlator \( \tilde{K}_{mn}(t, t') \) has a short correlation time \( \tau_{nm} \) given by equation (D36). With the assumption that the time evolution of the operator \( \Lambda_{mn}(t) \) is slow on the time scale \( \tau_{nm} \), in appendix E we derive the following master equation for the probability distribution \( P_n \) of the system (74):

\[ P_n + \Gamma_n P_n = \sum_m \Gamma_{mn} P_m, \]

(79)

where \( \Gamma_n = \sum_m \Gamma_{mn} \) and

\[ \Gamma_{mn} = \int_{-\infty}^{+\infty} d\tau \ e^{i\omega mn \tau - a_{mn} f(\tau)} \{ b_{mn} K(\tau) + [\tilde{T}_{mm} - c_{mn}] \left[ \tilde{T}_{mm}^{*} - c_{mn}^{*} f(\tau) \right] \}. \]

(80)

Coefficients \( a_{mn} \), \( b_{mn} \), \( d_{mn} \) are defined by equation (49) and

\[ T_{mn} = T_{mn} - i\langle n|n\rangle - d_{mn} \tau, \]

(81)

where \( \tau \) is the total reorganization energy described in section 3.5. \( T_{mn} = \tilde{T}_{mn} \). All matrix elements of the system operators in equation (80) are taken at the running moment of time \( t \). The master equation (79) with the rates (80) can be considered as a generalization of the NIBA (non-interacting bilinear approximation) approach \([3, 29, 40]\) to the case of the multi-level quantum system and also to the case of not-so-small tunneling amplitudes and energy gaps.

The rate \( \Gamma_{nn} \) can be written in a form similar to the single-qubit expression (9) and also to the multiqubit rate \( \Gamma_{n} \) given by equation (5) from [28] and by equation (68) from [29].
\[ \Gamma_{mn} = \int_{-\infty}^{+\infty} d\tau \ e^{i\omega_{mn}\tau} e^{-i\omega_{mn}\tau} \frac{1}{W_{mn}} \left\{ (1 + i\omega_{\tau}) \frac{\sinh(\pi T\tau)}{\pi T\tau} \right\} \]

\[ \times \{ b_{mn} \tilde{f} (\tau) + \{ T_{mn} - c_{mn} g (\tau) \} \{ T_{mn} - c_{mn} g (\tau) \} \}. \]  

(82)

Here we use equations (43) and (C1) and introduce the following parameters:

\[ \varepsilon_{mn} = a_{mn} \varepsilon_L, \quad W_{mn}^2 = a_{mn} W^2, \quad \eta_{mn} = a_{mn}. \]  

(83)

Equation (82) is equivalent to equations (5) and (6) in [28] and equations (43), (52), (54), and (68) in [29] with two important differences. First, \( T_{mn} \) in (81) includes the term \( \langle m|\hat{n}\rangle \) which can take care of non-adiabatic transitions such as those in the Landau–Zener effect. Second, the rate (82) does not contain any polaron shifts in the definition of \( \omega_{mn} \). While polaron shift has little effect on the results obtained in [28, 29] due to the relatively large energy gap and small number of qubits, it can have significant effect on small gap multiqubit problems, such as the one studied in section 7, rendering a large disagreement with the experiment.

### 4.2. Applicability conditions

The master equation (79) have been derived in appendix E with the proviso that

\[ \Gamma_{mn} T_{mn} \ll 1, \]  

(84)

where \( \Gamma_{mn} \) is the relaxation rate (80). The inverse correlation time of the bath, \( T_{mn}^{-1} \), is estimated in appendix D as the maximum of two parameters: the average energy distance \( |E_m - E_n| \) between the states \( |m\rangle \) and \( |n\rangle \) and the MRT linewidth \( W_{mn} = W\sqrt{a_{mn}} \),

\[ \frac{1}{T_{mn}} = \max \{ |E_m - E_n|, W_{mn} \}. \]  

(85)

It should be emphasized that we work in an arbitrary basis formed by the time-dependent states \( |\eta(t)\rangle \). The specific basis is chosen in view of the requirement that the perturbation parameter \( \Gamma_{mn} T_{mn} \) is much less than one. In the systems with ultra-small energy gaps the characteristic time \( T_{mn} \) calculated in the instantaneous energy basis goes to infinity since both energy parameters, the gap \( E_m - E_n \) and the linewidth \( W_{mn} \), tend to zero. In this basis the parameter \( \Gamma_{mn} T_{mn} \) is extremely large, and our perturbation treatment is not valid. The situation can be improved by going to another, so-called pointer basis [41], as we do in section 7.

### 5. Relaxation rate as a convolution of Bloch–Redfield and Marcus envelopes

In this section we show that, in addition to the expression (82) of the rate \( \Gamma_{mn} \) as the integral over time, the same rate can be conveniently represented as a convolution integral over frequencies of the Gaussian envelope multiplied by the Lorentzian function. As in the case of a single qubit described in section 2, the Gaussian curve is produced by LF bath noise. The Lorentzian factor is due to effects of the HF environment. Here, our aim is a generalization of the MRT single-qubit formula (17) to the multiqubit case where both, LF noise and the single-qubit tunneling, can be large.

#### 5.1. Convolution form of the rate \( \Gamma_{mn} \)

Using integration by parts and \( f (\tau) = ig (\tau) \), we obtain

\[ \int d\tau \ e^{i\omega_{mn}\tau} e^{-a_{mn} f (\tau)} g (\tau) = \frac{\omega'}{a_{mn}} \int d\tau \ e^{i\omega_{mn}\tau} e^{-a_{mn} f (\tau)}, \]

and

\[ \int d\tau \ e^{i\omega_{mn}\tau} e^{-a_{mn} f (\tau)} g^2 (\tau) = \int d\tau \ e^{i\omega_{mn}\tau} e^{-a_{mn} f (\tau)} \left[ \left( \frac{\omega'}{a_{mn}} \right)^2 - \frac{1}{a_{mn}} \tilde{f} (\tau) \right]. \]

Equation (80) can therefore be represented as

\[ \Gamma_{mn} = \int d\tau \ e^{i\omega_{mn}\tau} e^{-a_{mn} f (\tau)} \left[ b_{mn} - \frac{[\epsilon_{mn}]^2}{a_{mn}} \tilde{f} (\tau) + \frac{T_{mn} - \omega_{mn} \epsilon_{mn}}{a_{mn}^2} \right]. \]  

(86)

Let us introduce Fourier transformations

\[ G_{mn} (\omega) = \int_{-\infty}^{+\infty} d\tau \ e^{i\omega_{\tau} f (\tau)}, \]

(87)

where \( \mu = L, H \) for low and HF noise, respectively. Our goal is to write (86) as a convolution of the two functions \( G_{mn} (\omega) \) and \( G_{mn} (\omega) \). The integrand of equation (86) contains a term \( e^{-a_{mn} f (\tau)} \), which can be written in the following form,
\( e^{-a_m f (\tau)} = e^{-a_{mn} f(\tau)} e^{-a_{mn} f_m(\tau)} = \int \frac{d\omega_1}{2\pi} \int \frac{d\omega_2}{2\pi} e^{-i(\omega_1 + \omega_2) \tau} G_{mn}^L(\omega_1) G_{mn}^H(\omega_2). \)

Substituting in (86) and taking the integral over \( \tau \), we obtain:

\[ \Gamma_{nm} = \int \frac{d\omega}{2\pi} \Delta_{mn}^2(\omega) G_{mn}^L(\omega_{mn} - \omega) G_{mn}^H(\omega), \]  

where

\[ \Delta_{mn}^2(\omega) = |A_{mn}|^2 + B_{mn}(\omega^2 + W_{mn}^2), \]

and

\[ A_{mn} = \mathcal{F}_{mn} - \omega_{mn} \mathcal{C}_{mn}, B_{mn} = \frac{a_{mn} b_{mn} - |c_{mn}|^2}{a_{mn}^2} \left( \sum_{\alpha\beta} (\sigma_m^\alpha - \sigma_n^\alpha) \sigma_m^\beta - (\sigma_m^\beta - \sigma_n^\beta) \sigma_m^\alpha \right). \]

Here, we have used \( \mathcal{F}_n = W^2 + \mathcal{F}_H \) and neglected \( \mathcal{F}_H^2 \), which is \( O(\eta^2) \) in the weak-coupling approximation. Notice that \( B_{mn} \) is always positive and disappears in a single-qubit case where \( \alpha = \beta = 1 \). Also, we have \( A_{nn} = A_{nm} \) and \( B_{nn} = B_{mn} \).

Appendix F shows that the LF function \( G_{mn}^L(\omega) \) has a Gaussian shape,

\[ G_{mn}^L(\omega) = \sqrt{\frac{2\pi}{W_{mn}^2}} \exp \left[ - \frac{(\omega - \epsilon_{mn})^2}{2W_{mn}^2} \right]. \]

A similar line shape describes the rate of MRT in a system of qubits [25]. The HF component \( G_{mn}^H(\omega) \) can be approximated by a Lorentzian form, combining both Bloch–Redfield and Markovian rates:

\[ G_{mn}^H(\omega) = \frac{a_{mn}}{\omega^2 + \gamma_{mn}^2}. \]

The parameter \( \gamma_{mn} = \frac{a_{mn}}{2} S_{21}(0) \) does not depend on frequency \( \omega \). It follows from equation (44) that \( S_{21}(0) = \eta T \).

6. Special cases

In this section we verify detailed balance conditions for the equilibrium distribution of qubits and also consider the Bloch–Redfield and Marcus limits of the rates (88). In addition, we apply the results of the previous section to a single qubit interacting with a hybrid environment.

6.1. Equilibrium condition

We conclude from equations (88) and (F7) that

\[ \Gamma_{nm} = \exp \left( - \frac{\omega_{mn}}{T} \right) \Gamma_{nm}, \]

where \( \omega_{mn} \) is defined by equations (46) and (66). It follows from equation (79) that the equilibrium probabilities \( P_{eq}^n \) and \( P_{eq}^n \) to observe the qubits in the states \( |n\rangle \) and \( |m\rangle \), respectively, obey the equation:

\[ \sum_m (\Gamma_{nn} P_{eq}^n - \Gamma_{nm} P_{eq}^m) = 0. \]

The solution of this equation follows the detailed balance condition:

\[ \frac{P_{eq}^n}{P_{eq}^m} = \exp \left[ - \frac{E_m - E_n}{T} \right] \]

with the local energy levels \( E_n \) and \( E_n \) (46) and the bath temperature \( T \). Although there seems to be a freedom of choice in selecting the basis \( |n\rangle \), in reality equilibrium is established in the pointer basis [41], the basis which is most stable under environmental perturbations. We get back to this point in section 7.1.

The set of master equation (79) with the rates \( \Gamma_{nm} \) given by equation (88) provides a description of the dissipative dynamics of a quantum annealer during the entire annealing process. This description should be complemented by the equation for the off-diagonal elements \( \rho_{nm} \) of the system density matrix. The time evolution of \( \rho_{nm} \) is approximately described by the formula

\[ \rho_{nm} = e^{i \omega_{nm} t} \left( \langle S_{nm}^r S_{nm}^l \rangle(t) \right) \text{Tr}_S (\rho_S(0) \langle \Lambda_{nm}(t) \rangle) \simeq e^{i \omega_{nm} t} \left( \langle S_{nm}^r(t) S_{nm}^l(t) \rangle \right) \text{Tr}_S (\rho_S(0) \langle \Lambda_{nm}(0) \rangle). \]

To derive this relation, we start with equation (72) and move out the dephasing factor \( \langle S_{nm}^r(t) S_{nm}^l(t) \rangle(t) \). To obtain the first line of equation (96) we neglect terms proportional to pairings between the operators \( S_{nm}^r S_{nm}^l \) and the other operators \( U_j, U_l, A_{nm} \) involved in equation (72). These terms are determined by correlators of the off-diagonal
bath variables \( \dot{Q}_{mn} \) (64), which are assumed to be small. In the second line of equation (96) we replace the average \( \langle A_{mn}(t) \rangle \) by its value taken at the initial moment of time. This can be done since the time scale \( \Gamma_{mn}^{-1} \) of the function \( \langle A_{mn}(t) \rangle \) is much longer than the correlation time \( \tau_{\text{cor}} \) (83) of the prefactor in equation (96). Here we take into account the fact that, within the validity of our approach, we have two possibilities: in the first case the energy gap between states \( |m \rangle \) and \( |n \rangle \) is large, therefore the factor \( e^{i\omega_{mn}t} + e^{-i\omega_{mn}t} \) rapidly oscillates in time; in the second case the factor \( \langle S_{mn}^H(t) S_{n}(t) \rangle \), which is given by equation (D19), is the fast-decaying function of time. Equation (96) describes fast dephasing of the system of qubits.

6.2. Bloch–Redfield and Marcus limits

For the qubits weakly interacting with the HF noise in the absence of LF noise, the parameters of the LF bath go to zero: \( W = 0 \), \( \varepsilon_L = 0 \). The Gaussian envelope \( G_{mn}(\omega) \) (91) is approximated by the function \( 2\pi\delta(\omega) \), and the rate \( \Gamma_{mn} \) (88) takes the form

\[
\Gamma_{mn}^R = \Delta_{mn}^2(\omega_{mn}) \frac{a_{mn} S_{H}(\omega_{mn})}{\omega_{mn}^2 + \frac{1}{\Gamma_{mn}^2}}.
\]  

At large separation \( \omega_{mn} \) between the energy levels \( E_m \) and \( E_n \), we find that

\[
\Delta_{mn}^2(\omega_{mn}) = \frac{b_{mn}}{a_{mn}} \omega_{mn}^2.
\]

It is evident from equation (97) that, at \( |\omega_{mn}| \gg \gamma_{mn} \), the relaxation rate \( \Gamma_{mn} \) is proportional to the noise spectrum \( S_{H}(\omega_{mn}) \).

\[
\Gamma_{mn}^R = b_{mn} S_{H}(\omega_{mn}),
\]  

with the coefficient \( b_{mn} = \sum_{n=1}^{N} |\langle m|\sigma_3^n|n \rangle|^2 \), as it should be for the Bloch–Redfield rate. Transitions between states \( |m \rangle \) and \( |n \rangle \) separated by a zero Hamming distance (\( a_{mn} = 0 \)) are also described by the Redfield rate (98).

In the absence of HF noise, with \( \eta = 0 \) and \( S_H = 0 \), the function (92) peaks at zero frequency: \( G_{mn}(\omega) = 2\pi\delta(\omega) \). In this case the relaxation rate (88) of the many-qubit system is determined by the Gaussian line shape,

\[
\Gamma_{mn}^M = \Delta_{mn}^2(0) \sqrt{\frac{2\pi}{W_{mn}}} \exp \left[ -\frac{(E_m - E_n - \varepsilon_{mn})^2}{2W_{mn}^2} \right].
\]

This line shape is typical of the Marcus formulas [25, 30]. The multiqubit tunneling amplitude is determined by the expression

\[
\Delta_{mn}^2(0) = \left( b_{mn} - \frac{|c_{mn}|^2}{a_{mn}} \right) W^2 + \left[ T_{mn} - i \langle m|\sigma_3 |n \rangle - d_{mn} \varepsilon_L - \omega_{mn} \frac{c_{mn}}{a_{mn}} \right]^2.
\]

6.3. Relaxation rate of the single qubit

We assume that the single qubit is described by a Hamiltonian (2),

\[
H_S = -\frac{h}{2} \sigma_z - \frac{\Delta}{2} \sigma_z,
\]

with a bias \( h \), a tunneling amplitude \( \Delta \), and energy splitting \( \Omega_0 = \sqrt{\Delta^2 + h^2} \). The energy basis \( \{|k\} \) has only two states, \( |1 \rangle \) and \( |2 \rangle \). These states can be found from the equation: \( H_S|m \rangle = \Omega_m|m \rangle \). In equation (88) for the rate \( \Gamma_{mn} \) we put \( n = 1 \) and \( m = 2 \). The ground state \( |1 \rangle \) and the first excited state \( |2 \rangle \) have the energies:

\[ E_m = -E_n = \Omega_0/2. \]

We work in the energy basis where \( T_{mn} = 0 \). For the single qubit we obtain the following set of parameters,

\[
a_{mn} = 4 \frac{h^2}{\Omega_0^2}, \quad b_{mn} = \Delta^2 \frac{\Omega_0^2}{\Omega_0^2}, \quad c_{mn} = -2 \frac{h\Delta}{\Omega_0^2}, \quad d_{mn} = 0,
\]

so that \( B_{mn} = 0 \) and \( \Delta_{mn}^2(\omega) = \Delta^2/a_{mn} \) (see sections 3.6 and 5.1 for definitions). It follows from equation (88) that in the case of hybrid noise the single-qubit relaxation rate combines both, Bloch–Redfield and Marcus, formulas,

\[
\Gamma_{mn} = \Delta^2 \int \frac{d\omega}{2\pi} \frac{S_{H}(\omega)}{\omega^2 + \frac{\Gamma_{mn}^2}{2a_{mn} W^2}} \exp \left[ -\frac{2\pi}{a_{mn} W^2} \frac{\Gamma_{mn}^2}{2a_{mn} W^2} \left( \frac{\Omega_0 - \omega - \varepsilon_L}{2a_{mn} W^2} \right)^2 \right],
\]

where \( \gamma_{mn} = \frac{a_{mn} W^2}{2}. \) In the limit of small \( \Delta \) (and at positive \( h \), for example) we have \( \Omega_0 = h, a_{mn} = 4 \). In this case the rate (102) turns into equation (17) shown in section 2. The master equation (79), with the single-qubit rate (102), is valid if
as it follows from equations (85) and (101). The condition (103), which is written in the energy basis, fails near the degeneracy point, \( h = 0 \), at a small tunneling amplitude \( \Delta \). In order to keep our theory alive we have to move to the computation basis formed by eigenstates of \( \sigma_z \)-matrix.

7. Dissipative evolution of a 16 qubit system

In this section we analyze dynamics of the 16 qubit system with the set of couplings and biases determined by the Dickson instance (see figure 1). This instance was proposed in [42] and investigated in details in [33]. The energy spectrum of the problem features an extremely small gap between the ground and first excited states. The existence of such a gap presents a computational bottleneck for QA. An experimental technique to overcome this difficulty by individual tuning qubit’s transverse fields has been demonstrated in [43]. Nevertheless, a theoretical analysis of dissipative dynamics in this system presents a real challenge.

The probability distribution of the qubits is governed by the master equation (79) with the relaxation matrix given by equation (88). The qubits are described the Hamiltonian (18). In the problem Hamiltonian (19) we have ferromagnetic couplings between qubits, \( J_{ij} = -1 \), for every pair of coupled qubits. Two internal qubits have zero biases, \( h_{i4} = h_{10} = 0 \), whereas the other internal qubits are negatively biased, with

\[
\begin{align*}
\Gamma_{11} & = h_1 = h_2 = h_3 = h_6 = h_{11} = h_{12} = -1. \\
\text{All external qubits have positive biases:} & \\
& h_4 = h_5 = h_7 = h_8 = h_{13} = h_{14} = h_{15} = h_{16} = 1.
\end{align*}
\]

We use the annealing curves \( \Delta_A(s) = \Delta_0 A(s) \) and \( B(s) \) plotted in figure 2. This annealing schedule, which is taken from [33], has minor variations between the qubits. These variations, although not so important, allow us to reproduce the same extremely small energy gap, \( E_2 - E_1 = 0.011 \) mK, between the ground and the first excited states as in experiments performed in [33]. The gap is located at \( s^* = 0.6396 \). In figure 3 we show the four lowest energy levels of the system near the anticrossing. The most interesting annealing dynamics happen in the interval \( s_1 < s < s_2 \), where \( s_1 = 0.625 \) and \( s_2 = 0.65 \).

The two states with the lowest energies, \( |\text{GM}\rangle \) and \( |\Sigma\rangle \), are given by the expressions

\[
|\text{GM}\rangle = |\uparrow_1 \downarrow_2 \uparrow_3 \downarrow_4 \downarrow_5 \downarrow_6 \downarrow_7 \uparrow_8 \downarrow_9 \downarrow_{10} \downarrow_{11} \downarrow_{12} \rangle \otimes |\downarrow_{13} \downarrow_{14} \downarrow_{15} \downarrow_{16} \rangle,
|\Sigma\rangle = |\uparrow_1 \uparrow_2 \uparrow_3 \uparrow_4 \uparrow_5 \uparrow_6 \uparrow_7 \uparrow_8 \uparrow_9 \uparrow_{10} \uparrow_{11} \uparrow_{12} \rangle \otimes |\downarrow_{13} \downarrow_{14} \downarrow_{15} \downarrow_{16} \rangle.
\]

Here we introduce the eigenstates \( |\uparrow_\alpha\rangle \) and \( |\downarrow_\alpha\rangle \) of the matrix \( \sigma_z^\alpha \), and also their superposition \( |\pm_\alpha\rangle \),

\[
\sigma_z^\alpha |\uparrow_\alpha\rangle = |\uparrow_\alpha\rangle, \quad \sigma_z^\alpha |\downarrow_\alpha\rangle = -|\downarrow_\alpha\rangle,
|\pm_\alpha\rangle = \frac{1}{\sqrt{2}} (|\uparrow_\alpha\rangle \pm |\downarrow_\alpha\rangle).
\]

More details can be found in [33] and in the supplementary information for that paper. It follows from figure 2(c) of [33] that, before the anticrossing at \( s < s^* \), the instantaneous eigenstates of the 16 qubit system...
coincide with the diabatic states: $|1\rangle = |\Sigma\rangle$, $|2\rangle = |\Gamma M\rangle$. After the anticrossing point at $s > s^*$, we have the reverse situation, with $|1\rangle = |\Gamma M\rangle$ and $|2\rangle = |\Sigma\rangle$. Although the experimental results provided in [33] were in accordance with the physical intuition given in the paper, no theoretical analysis was provided. This was due to the lack of an open quantum theory that takes into account both LF and HF noises. Here, we apply our approach to provide a theoretical explanation of the experimental results of [33].

The presence of a very small gap and the time-dependence of the system Hamiltonian, which becomes nonadiabatic near the minimum gap, make the problem instance in figure 1 difficult to analyze within one theoretical framework in all regions during the annealing. As such, some tricks are necessary to choose the proper basis as we discuss next.

### 7.1. Rotation of the basis

The dissipative dynamics of the qubits coupled to a heat bath is described by the master equation (79). These equations are derived with the proviso that the rate $\Gamma_{nm}$ of the relaxation (88) between the states $|n\rangle$ and $|m\rangle$ is much less than the inverse time scale $\tau_{mn}^{-1}$ given by equation (85), so that: $\Gamma_{nm} \tau_{mn} \ll 1$. For the system of 16 qubits under study the perturbation requirement breaks down at the anticrossing point as it is evident from figure 4(a). Here we plot the energy gap, $E_2 - E_1$, between two instantaneous eigenstates of the Hamiltonian $H_S$ (see dot-dashed blue line), and also the MRT line width, $W_{21} = a_{21} W$ (see continuous green line), as functions of the annealing parameter $s$. At $s = s^*$ both parameters, $E_2 - E_1$ and $W_{21}$, become extremely small, leading to a diverging correlation time $\tau_{mn}$ (85). At the same time, $\Gamma_{12}$ becomes very large due to the contribution from $\tilde{T}_{21}$.  

Figure 2. Annealing parameters $B(s)$ (black line) and tunneling amplitudes $\Delta_1(s), \ldots, \Delta_{16}(s)$ (all other colors) plotted as functions of $s$.

Figure 3. Four energy levels of the 16 qubit system as functions of the annealing parameter near the anticrossing of two lowest energy levels. Energies are counted from the energy $E_1$ of the ground state.
Both of these break the applicability condition (84) in the instantaneous energy basis. Moreover, in this basis the time dependence of the Hamiltonian can create nonzero off-diagonal elements of the density matrix near the minimum gap due to nonadiabatic transitions. These terms do not decay quickly as required by our theory. As we shall see, all these issues can be resolved by rotating the basis. This is equivalent to the introduction of the pointer basis as described in [28, 29, 41]. We rotate the two anticrossing states as:

\[ 1' = \cos \Theta |1\rangle + \sin \Theta |2\rangle, \]
\[ 2' = -\sin \Theta |1\rangle + \cos \Theta |2\rangle. \] (105)

The rotation angle \( \Theta \) can depend on the annealing parameter \( s \) and therefore on time \( t \). For real eigenstates \( |1\rangle \) and \( |2\rangle \) it follows that

\[ \langle 2' | \frac{d}{ds} | 1' \rangle = \langle 2 | \frac{d}{ds} | 1 \rangle + \frac{d\Theta}{ds}. \] (106)

We choose the rotation angle \( \Theta(s) \) such that in the rotated basis

\[ \langle 2' | \frac{d}{ds} | 1' \rangle = 0. \] (106)

This means that the \( s \)-dependence of the angle \( \Theta \) is determined by

\[ \frac{d\Theta}{ds} = \frac{\langle 2 | \frac{dH}{dt} | 1 \rangle}{E_2 - E_1}. \] (107)

Notice that (106) assures minimum quantum transitions between the two states \( |1'\rangle \) and \( |2'\rangle \) near the anticrossing and therefore minimum generation of off-diagonal elements of the density matrix. As we show in section 7.2, it also resolves all issues with the applicability condition (84) discussed above. It should be mentioned that here the rotation angle \( \Theta \) is different from the rotation angle \( \theta_k \) of the pointer basis in [28, 29], where \( \theta_k \) maximizes the parameter \( W_{12} \) calculated for the states under consideration (see, for example, equations (30), (32) in [29]). In our case the angle \( \Theta \) minimizes the Landau–Zener transitions between two anticrossing states. Recall that in [28, 29] the Landau–Zener transitions are just neglected.

A solution of equation (107) is shown in figure 4(c). In the beginning of annealing \( \Theta \approx 0 \), so that the rotated basis coincides with the instantaneous basis. Near the anticrossing point, at \( s = s^* \), the angle \( \Theta \) rapidly switches to \( \pi/2 \). We notice that, with the condition (106), the renormalized matrix element \( \tilde{T}_{1'1'}(68) \) is

\[ \tilde{T}_{1'1'} = \langle 2' | H_{1'1'} | 1' \rangle = \frac{E_2 - E_1}{2} \sin 2\Theta. \] (108)

This is zero before \( (\Theta = 0) \) and after \( (\Theta = \pi/2) \) the anticrossing due to the sine function and is very small at the anticrossing due to the small gap \( (E_2 - E_1 \approx 0) \). This means that \( \tilde{T}_{1'1'} \) does not contribute to the rate \( \Gamma_{1'2'} \), keeping
it small, within the applicability range of our model. For this example we rotate only the two lowest-energy states that have an anticrossing. However, the rotation can be applied to anticrossing excited states as well, if necessary.

7.2. Rates and probabilities for the 16 qubit system

In this section we calculate the rate $G_{12}$ (88) of the system relaxation between the states $|1\rangle$ and $|0\rangle$. These states are defined as superpositions (105) of the instantaneous ground and first excited states. The rotation angle $\Theta(s)$ is chosen as the solution of equation (107). Hereafter we drop primes from the state number and use $\Gamma_{12}$ instead of $G_{12}$. I n figures 5(a), 6(a), and 7(a) we show the $s$-dependence of the hybrid relaxation rate $\Gamma_{12}$ (black line) in comparison to the Marcus rate (blue dashed line) and to the Bloch–Redfield rate (red dashed line). The Bloch–Redfield rate is calculated with equation (97), whereas the Marcus rate is given by equation (99). To verify our approach, in figures 5(b), 6(b), and 7(b) we show the evolution of the supposed-to-be small parameter $\Gamma_{12} \times \tau_{12}$ (84) during the annealing process. Recall that all rates and parameters are written in the rotated basis (105). We keep the same temperature, $T = 10$ mK, in every figure. We change, however, the coupling constant $\eta$ and the MRT line width $W$, thus changing a relative contribution of the HF bath and the LF environment to the hybrid.

Figure 5. (a) At large coupling to the HF bath ($\eta = 0.25$) and at a small interaction with the LF noise ($W = 2$ mK), the hybrid rate $\Gamma_{12}$ is close to the Bloch–Redfield rate $R_{12}$. (b) The perturbation parameter $\Gamma_{12} \tau_{12}$ is less than 0.3.

Figure 6. (a) When both couplings are large ($\eta = 0.25$ and $W = 10$ mK), the hybrid rate $\Gamma_{12}$, taken along the annealing path, deviates from Bloch–Redfield, $R_{12}$, and from Marcus, $M_{12}$, rates. (b) The perturbation parameter is small, $\Gamma_{12} \tau_{12} < 0.04$. 
The perturbation parameter remains low during the annealing process, $\Gamma_{12} \tau_{21} < 0.3$. In figure 6 we consider the intermediate case where qubit couplings to both LF and HF environments are quite large, so that $\eta = 0.25$ and $W = 10$ mK. Here, the hybrid rate $\Gamma_{12}$ differs from the Redfield rate $\Gamma_{12}^R$ and from the Marcus rate $\Gamma_{12}^M$. The perturbation parameter is decreasing: $\Gamma_{12} \tau_{21} \approx 0.04$. The hybrid rate $\Gamma_{12}$ almost coincides with the Marcus rate $\Gamma_{12}^M$. The validity of these results is verified by the small parameter $\Gamma_{12} \tau_{21} < 0.008$ shown in figure 7(b).

In figure 8, in parallel with the energy spectrum, we plot a time dependence of the probabilities $P_1$ and $P_2$ to find the 16 qubit system in the instantaneous energy eigenstates |1\rangle and |2\rangle of the Hamiltonian $H_S$ (18). To calculate these probabilities, we obtain the numerical solution of the master equation (79) for the probabilities $P_1$ and $P_2$ to observe the system in the states |1\rangle and |2\rangle (105). After that, we rotate the basis back, to the instantaneous energy eigenstates |1\rangle and |2\rangle. The contribution of the off-diagonal elements of the density matrix to the probabilities $P_1$ and $P_2$ rapidly disappears as it follows from equations (96) and (D19). We also show the

Figure 7. (a) At sufficiently large coupling of the system to the low-frequency bath, where $W = 10$ mK, and at small coupling to the high-frequency bath, with $\eta = 0.1$, the hybrid rate $\Gamma_{12}$ is close to the Marcus expression $\Gamma_{12}^M$. (b) The perturbation parameter is decreasing in this case: $\Gamma_{12} \tau_{21} < 0.01$.

Figure 8. (a) Instantaneous energy spectrum of the 16 qubit system near the anticrossing point. (b) The evolution of the probabilities $P_1, P_2$ to find the system in the instantaneous energy eigenstates during the annealing process at the total anneal time $t_f = 2$ ms and at $\eta = 0.1$, $W = 10$ mK, $T = 10$ mK. We also show the time evolution of the probability $P_{GM}$ for the system to be in the |GM\rangle.
evolution of the probability $P_{\text{GM}}$ (blue curve) to find the system in the state $\ket{\text{GM}}$ defined in (104). Here, we have a qualitative agreement with the experimental results shown in figure 2(d) of [33]).

7.3. Thermal enhancement of the success probability

The goal of annealing is to reach the ground state at the end of the evolution. It follows from figure 2(c) of [33] that at the end of annealing, at $t = t_f$ the ground state of the 16 qubit system coincides with the state $\ket{\text{GM}}$ shown in equation (104). We therefore define the success probability as the probability $P_{\text{GM}}$ to observe the system in $\ket{\text{GM}}$ at $t = t_f$. Figure 3 of [33] demonstrates the temperature dependence of $P_{\text{GM}}$. It is clear from this figure that, at sufficiently fast annealing ($t_f \lesssim 100 \text{ ms}$), $P_{\text{GM}}$ grows with increasing temperature from 20 to 40 mK and decreases after. Our goal is to reproduce this non-monotonic behavior with our open quantum model. It should be noted that we do not aim to precisely fit the experimental data to the results of our model.

We solve numerically the master equation (79) with the relaxation rates given by the convolution formula (88) written in the rotated basis (105). We perform simulation for the total anneal time $t_f$ between 0.04 and 4 ms. An example of $P_{\text{GM}}(t_f)$ as a function of time is shown in figure 8(b) in the section 7.2. Figure 9 plots the success probability, $P_{\text{GM}}(t_f)$, as a function of temperature $T$ for different speeds of annealing characterized by the anneal time $t_f$. In the theoretical calculations we assume that $\eta = 0.1$ and $W = 20 \text{ mK}$. Figure 9 reproduces the results shown in figure 3 of [33], including the enhancement $P_{\text{GM}}$ at low temperatures and its reduction at $T \gtrsim 40 \text{ mK}$. As mentioned in [33], this decrease may be related to the excitation of the high-energy levels separated from the two lowest states by a gap of order 40 mK (see the spectrum in figure 3).

8. Conclusions

In this paper, we have derived a set of master equations describing a dissipative evolution of an open quantum system interacting with a complex environment. The environment has low-frequency and high-frequency components, as in the case of realistic qubits affected by the hybrid bath, which includes $1/f$ and Ohmic noise. A part of the system–bath interaction is treated in a nonperturbative way. This mathematical treatment allows us to combine the Bloch–Redfield and Marcus approaches to the theory of open quantum systems and obtain the relaxation rates, which are well-suited for the description of dissipative dynamics of many-qubit quantum objects, such as quantum annealers, in the whole annealing range.

The relaxation rates are expressed in the convenient convolution form clearly showing the interplay between the low- and high-frequency noise. The main results of the paper are given by the master equation (79) with the relaxation rates (88). As an illustration, we apply the theory to the 16 qubit quantum annealer investigated in [33]. The instance studied there features an extremely small gap between the ground and first excited states. With the proper rotation of the basis, we have solved the master equations and theoretically confirmed the main experimental findings of [33]. The results of the paper may be useful for understanding a dissipative evolution of various systems, from chromophores in quantum biology [30–32] to qubits in real-world quantum processors [14, 15, 44].

Figure 9. End-of-annealing probability to be in the $\ket{\text{GM}}$ state, $P_{\text{GM}}$ as a function of temperature $T$ and the anneal time $t_f$ at $\eta = 0.1$ and $W = 20 \text{ mK}$. 
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Appendix A. Notations

In this appendix we assemble notations used throughout the paper, so that the main part of the paper becomes easier to follow. In a chosen basis \( \{|n\rangle \} \) the matrix elements of the system Hamiltonian \( H_S \) (18) and those of the Pauli matrix \( \sigma_z^\alpha \) of the \( \alpha \)-qubit are denoted as

\[
E_n = \langle n | H_S | n \rangle, \quad T_{mn} = \langle m | H_S | n \rangle, \\
\sigma_z^\alpha_n = \langle n | \sigma_z^\alpha | n \rangle, \quad \sigma_z^{\alpha m} = \langle m | \sigma_z^\alpha | n \rangle.
\]  

(A1)

For combinations of the matrix elements we introduce the following notations:

\[
a_{mn} = \sum_\alpha (\sigma_m^\alpha - \sigma_n^\alpha)^2, \quad b_{mn} = \sum_\alpha |\sigma_m^\alpha|_2, \\
c_{mn} = \sum_\alpha \sigma_m^\alpha (\sigma_m^\alpha - \sigma_n^\alpha), \quad d_{mn} = \sum_\alpha \sigma_m^\alpha (\sigma_m^\alpha + \sigma_n^\alpha).
\]  

(A2)

The parameters of the bath are defined as

\[
\varepsilon_L = \int \frac{d\omega}{2\pi} \frac{S_L(\omega)}{\omega}, \quad \varepsilon_H = \frac{\eta \omega_c}{2\pi}, \quad \varepsilon = \varepsilon_L + \varepsilon_H, \\
W^2 = \int \frac{d\omega}{2\pi} S_L(\omega) = 2 \varepsilon_L T,
\]

(A3)

with \( \eta \) and \( \omega_c \) defined in section 3.5. We also introduce

\[
\varepsilon_{mn} = a_{mn} \varepsilon_L, \quad W_{mn}^2 = a_{mn} W^2, \\
\eta_{mn} = a_{mn} \eta, \quad \gamma_{mn} = \frac{1}{2} \eta_{mn} T. 
\]

(A4)

For a time-dependent basis \( |n(t)\rangle \), we write the following functions of time:

\[
\omega_{mn}(t) = E_m(t) - E_n(t), \\
\phi_{mn}(t) = \int_0^t d\tau \omega_{mn}(\tau), \\
\tilde{T}_{mn} = T_{mn} - i \langle m | n \rangle, \\
\tilde{T}_m = T_m - i \langle m | n \rangle - d_{mn} \varepsilon.
\]

(A5)

The coefficients \( A_{mn}, B_{mn} \) used in equations (88) and (89) are defined as

\[
A_{mn} = \frac{\tilde{T}_{mn} - \omega_{mn} c_{mn}}{a_{mn}} \quad B_{mn} = \frac{am b_{mn} - |c_{mn}|^2}{a_{mn}^2} \\
= \frac{1}{2a_{mn}^2} \sum_{\alpha, \beta} |(\sigma_m^\alpha - \sigma_n^\alpha) \sigma_{mn}^\beta - (\sigma_m^\beta - \sigma_n^\beta) \sigma_{mn}^\alpha|^2.
\]

(A6)

Appendix B. A specific example of a heat bath

A Gaussian heat bath can be modeled as a collection of independent harmonic oscillators \([3, 31]\) with the Hamiltonian

\[
H_B = \sum_j \left( \frac{p_j^2}{2m_j} + \frac{m_j \omega_j^2 x_j^2}{2} \right).
\]

(B1)

Oscillators are characterized by positions \( x_j \) and momenta \( p_j \) and also by the set of mass, \( m_j \), and frequencies, \( \omega_j \). For this specific example the bath operator \( Q \) is a linear superposition of coordinates \( x_j \):

\[
Q = \sum_j \lambda_j m_j \omega_j^2 x_j.
\]

(B2)
The coupling parameter $\lambda_j$ is proportional to the displacement of the position of the $j$-oscillator caused by the flipping of the qubit. For this model, the spectrum of the bath fluctuations (3),

$$S(\omega) = \chi''(\omega) \left[ \coth \left( \frac{\omega}{2T} \right) + 1 \right],$$

is proportional to the imaginary part of the bath susceptibility, $\chi''(\omega)$, which defines dissipative properties of the bath,

$$\chi''(\omega) = \pi \sum_j m_j \omega_j^3 \lambda_j^2 \left[ \delta(\omega - \omega_j) - \delta(\omega + \omega_j) \right].$$

**Appendix C. HF dissipative functions**

For the ohmic HF bath characterized by the spectrum (44), the dissipative functions $f_H, g_H$, and a correlator $K_{H}$ are given by the formulas

$$f_H(t) = \frac{\eta}{2\pi} \ln \left( 1 + i \omega_c t \right) \frac{\sinh(\pi T t)}{\pi T t},$$

$$g_H(t) = \frac{\eta}{2\pi} \frac{\omega_c}{1 + kT} + i \frac{\eta T}{2} \left[ \coth(\pi T t) - \frac{1}{\pi T t} \right],$$

$$K_H(t) = \frac{\eta}{2\pi} \left( \frac{\omega_c}{1 + kT} \right)^2 - \frac{1}{\pi T t} \left[ \frac{\pi T}{\sinh(\pi T t)} \right]^2 + \frac{1}{t^2},$$

provided that the cutting frequency $\omega_c$ is much higher than the temperature, $\hbar \omega_c \gg k_B T$. We notice that at large times, $t \gg \frac{\hbar}{\pi k_B T}$, all the three functions vanish. In equation (44) we introduce $\eta$ as a small dimensionless coupling constant \[3\], and $\omega_c$ as a large cutting frequency of the HF noise. For the Ohmic bath, the spectral density $\chi''_{H}(\omega)$ is defined as

$$\chi''_{H}(\omega) = \frac{\eta \omega}{2} e^{-|\omega|/\omega_c}.$$

We assume independent noise sources coupled to every qubit, each described by the above-mentioned formulas with identical parameters.

**Appendix D. Correlator $\not K_{mn}^{m'n'} (t, t')$**

Here we calculate the correlator (70) of the nondiagonal bath variables with indexes $m \neq n$ and $m' \neq n'$. In this case, the bath operators are defined by equation (64), and the correlator $\not K_{mn}^{m'n'} (t, t')$ is given by the formula

$$\not K_{mn}^{m'n'} (t, t') = e^{i\Delta_{mn}(t)} e^{i\Delta_{m'n'}(t')} \langle S_m(t) S_{m'}(t') \rangle \langle S_{n'}(t') S_n(t) \rangle,$$

$$\times S_{m'}^+(t') \langle Q_{m'n'}(t') - \tilde{T}_{m'n'}(t') \rangle S_n(t') \rangle.$$  

(D1)

This correlator can be represented as a sum of four components:

$$\not K_{mn}^{m'n'} (t, t') = e^{-i \int_0^t \omega_{mn}(\tau) d\tau + i \int_0^t \omega_{m'n'}(\tau) d\tau} \{ (i) + (ii) + (iii) + (iv) \},$$

(D2)

with

$$(i) = \tilde{T}_{mn}^i \tilde{T}_{m'n'}^i \not F_{mn}^{m'n'} (t, t'),$$

$$(ii) = -\tilde{S}_{mn}^i (t) \tilde{S}_{m'}(t') \tilde{S}_{m'}^+(t') \langle Q_{m'n'}(t') \rangle,$$

$$(iii) = -\tilde{S}_{m'}^+(t') \langle Q_{mn}(t) \tilde{S}_{n}(t) \tilde{S}_{m'}^+(t') \rangle,$$

$$(iv) = \langle S_{m'}^+(t') \langle Q_{mn}(t) \tilde{S}_{n}(t) \tilde{S}_{m'}^+(t') \rangle S_n(t') \rangle.$$  

(D3)

where

$$\not F_{mn}^{m'n'} (t, t') = \langle S_{m'}^+(t') \tilde{S}_{n}(t) \tilde{S}_{m'}^+(t') \rangle.$$  

(D4)

The bath variable $Q_{mn}$ is defined in (47), and $\tilde{S}_n$ is the S-matrix of the bath given by equation (57).
D.1. Term (i) and the functional \(F_{mn}^{m'n'}\)

To calculate the functional \(F_{mn}^{m'n'} (t, t')\) (D4) we consider a more complicated term

\[
F_{mn}^{m'n'} (t, \tau, t', \tau') = \langle S^\dagger_m(t, \tau) S_n(t, \tau) S_{m'}(t', \tau') S_{n'}(t', \tau') \rangle,
\]

where the modified S-matrix of the bath, \(S_n(t, \tau)\), is defined by equation (61). We notice that

\[
F_{mn}^{m'n'} (t, t') = F_{mn}^{m'n'} (t, t'),
\]

The functional \(F_{mn}^{m'n'} (t, \tau, t', \tau')\) obeys two differential equations:

\[
\frac{d}{dt} F_{mn}^{m'n'} (t, \tau, t', \tau') = \sum_{\alpha} \sigma_{mn}^\alpha(t) \langle S^\dagger_m(t, \tau) Q_\alpha(t) S_n(t, \tau) S_{m'}(t', \tau') S_{n'}(t', \tau') \rangle,
\]

\[
\frac{d}{dt'} F_{mn}^{m'n'} (t, \tau, t', \tau') = \sum_{\alpha} \sigma_{mn}^\alpha(t') \langle S_{m'}(t', \tau') S_n(t, \tau) S^\dagger_m(t, \tau) Q_\alpha(t, \tau) S_{n'}(t', \tau') \rangle,
\]

where we introduce the notation \(\sigma_{mn}^\alpha(t) = \sigma_n^\alpha(t) - \sigma_m^\alpha(t)\). With the Wick theorem [45], we have to take all possible pairings of the Gaussian operators \(Q_\alpha(t)\) and \(Q_\alpha(t')\) in equation (D7) with other operators. As a result, we obtain

\[
\frac{d}{dt} \ln F_{mn}^{m'n'} (t, \tau, t', \tau') = \sum_{\alpha} \sigma_{mn}^\alpha(t) \langle S^\dagger_m(t, \tau) S_n(t, \tau) \rangle \int_0^\tau d\tau_1 \frac{d}{d\tau_1} K_m(\tau_1, \tau_2) - \langle S_{m'}(t', \tau') S_{n'}(t', \tau') \rangle \int_0^{\tau'} d\tau_1 \frac{d}{d\tau_1} K_m(\tau_1, \tau_2) \rangle,
\]

\[
\frac{d}{dt'} \ln F_{mn}^{m'n'} (t, \tau, t', \tau') = \sum_{\alpha} \sigma_{mn}^\alpha(t') \langle S^\dagger_m(t', \tau') S_n(t', \tau') \rangle \int_0^{\tau'} d\tau_1 \frac{d}{d\tau_1} K_m(\tau_1, \tau_2) - \langle S_{m'}(t, \tau) S_{n'}(t, \tau) \rangle \int_0^{\tau} d\tau_1 \frac{d}{d\tau_1} K_m(\tau_1, \tau_2) \rangle.
\]

The solution of these two equations is given by the expression

\[
\ln F_{mn}^{m'n'} (t, \tau, t', \tau') = -\sum_{\alpha} \sigma_{mn}^\alpha(t) \langle S_{m'}(t', \tau') S_{n'}(t', \tau') \rangle \int_0^\tau d\tau_1 \frac{d}{d\tau_1} K_m(\tau_1, \tau_2) \]

\[
+ \sum_{\alpha} \sigma_{mn}^\alpha(t) \langle S^\dagger_m(t, \tau) S_n(t, \tau) \rangle \int_0^\tau d\tau_1 \frac{d}{d\tau_1} K_m(\tau_1, \tau_2) \]

\[
+ \sum_{\alpha} \sigma_{mn}^\alpha(t') \langle S^\dagger_m(t', \tau') S_n(t', \tau') \rangle \int_0^{\tau'} d\tau_1 \frac{d}{d\tau_1} K_m(\tau_1, \tau_2) \]

\[
+ \sum_{\alpha} \sigma_{mn}^\alpha(t') \langle S_{m'}(t, \tau) S_{n'}(t, \tau) \rangle \int_0^{\tau} d\tau_1 \frac{d}{d\tau_1} K_m(\tau_1, \tau_2) \].
\]

It follows from equation (D6) that the functional \(F_{mn}^{m'n'} (t, t')\) of the Gaussian bath is described by the formula

\[
F_{mn}^{m'n'} (t, t') = \exp \left\{ -\sum_{\alpha} (\sigma_{mn}^\alpha - \sigma_{m'n'}^\alpha(t)) (\sigma_{m'n'}^\alpha - \sigma_{mn}^\alpha(t')) \right\}
\]

\[
\times \int_0^t d\tau_1 \int_0^{t'} d\tau_2 \frac{d}{d\tau_1} K_m(\tau_1, \tau_2) + \sum_{\alpha} (\sigma_{mn}^\alpha - \sigma_{m'n'}^\alpha(t)) \int_0^t d\tau_1 \int_0^{\tau_1} d\tau_2 \]

\[
\times \left[ \langle S^\dagger_m(t) K_m(\tau, \tau) \rangle K_m(t, \tau') - \sigma_{mn}^\alpha(t) K_m(t, \tau') \right] + \sum_{\alpha} (\sigma_{m'n'}^\alpha - \sigma_{mn}^\alpha(t')) \int_0^{t'} d\tau_1 \int_0^{\tau_1} d\tau_2 \]

\[
\times \left[ \langle S^\dagger_m(t') K_m(\tau, \tau) \rangle K_m(t, \tau') - \sigma_{m'n'}^\alpha(t') \right].
\]

Here \(K_m(t, \tau)\) is the correlation function (34) of the free bath.

D.2. Terms (ii) and (iii)

Using the Wick theorem [45], we find that the terms (ii) and (iii) are proportional to the correlators

\[
\langle S^\dagger_m(t) S_n(t) S^\dagger_{m'}(t') S_{n'}(t') \rangle = i \sum_{\alpha} \sigma_{mn}^\alpha(t) \langle S^\dagger_m(t) F_{mn}^{m'n'} (t, t') \rangle \]

\[
\times \left\{ \sigma_{m'n'}^\alpha(t') \int_0^t dt K_m(t, t') + \int_0^t dt' \frac{d}{dt} \left[ \sigma_{m'n'}^\alpha(t') K_m(t, t') - \sigma_{mn}^\alpha(t') K_m(t, t') \right] \right\},
\]

\[
\langle S^\dagger_m(t) Q_{mn}(t) S_n(t) S^\dagger_{m'}(t') S_{n'}(t') \rangle = i \sum_{\alpha} \sigma_{mn}^\alpha(t) \langle S^\dagger_m(t) F_{mn}^{m'n'} (t, t') \rangle \]

\[
\times \left\{ \sigma_{m'n'}^\alpha(t') \int_0^t dt K_m(t, t') + \int_0^t dt' \frac{d}{dt} \left[ \sigma_{m'n'}^\alpha(t') K_m(t, t') - \sigma_{mn}^\alpha(t') K_m(t, t') \right] \right\}.
\]

(D11)
D.3. Term (iv) and the total correlator

The last term in equation (D3) can be written as

\[
\langle S_{mn}(t) Q_{mn}(t) S_{mn}^\dagger(t) Q_{mn}^\dagger(t) \rangle = \sum_\alpha \sigma_{mn}^{\alpha}(t) \sigma_{mn}^{\alpha}(t') K_{\alpha}(t, t') F_{mn}^{\alpha\beta}(t, t') + i^2 \sum_\alpha \sigma_{mn}^{\alpha}(t) \sigma_{mn}^{\alpha}(t') F_{mn}^{\alpha\beta}(t, t')
\]

\[
\times \left\{ \int_0^{t'} dt \left[ \sigma_{nm}^{\alpha}(t) K_{\alpha}(t, t') - \sigma_{mn}^{\alpha}(t) K_{\alpha}(t, t') \right] + (\sigma_{nm}^{\alpha} - \sigma_{mn}^{\alpha})(t) \int_0^{t'} dt K_{\alpha}(t, t') \right\}
\]

\[
\times \left\{ \int_0^{t'} dt \left[ \sigma_{nm}^{\alpha}(t') K_{\alpha}(t', t) - \sigma_{mn}^{\alpha}(t') K_{\alpha}(t', t) \right] + (\sigma_{nm}^{\alpha} - \sigma_{mn}^{\alpha})(t) \int_0^{t'} dt K_{\alpha}(t', t) \right\}.
\]

The correlation function (D2) of the operators \( \hat{Q}_{mn}(t) \) and \( \hat{Q}_{mn}^\dagger(t') \) has the form

\[
\hat{K}_{mn}^{(i)}(t, t') = e^{i\phi_{mn}(t)} e^{i\phi_{mn}^\dagger(t')} \{ \hat{K}_{mn}^{(i)}(t, t') \}
\]

\[
+ U_{mn}^{(i)}(t, t') \hat{V}_{mn}^{(i)}(t, t') \} F_{mn}^{(i)}(t, t'),
\]

where

\[
\hat{K}_{mn}^{(i)}(t, t') = \sum_\alpha \sigma_{mn}^{\alpha}(t) \sigma_{mn}^{\alpha}(t') K_{\alpha}(t, t'), U_{mn}^{(i)}(t, t') = \hat{T}_{mn}(t)
\]

\[
- i \sum_\alpha \sigma_{mn}^{\alpha}(t) \left\{ \left( \sigma_{nm}^{\alpha} - \sigma_{mn}^{\alpha}(t') \right) \int_0^{t'} dt K_{\alpha}(t, t') + \int_0^{t'} dt K_{\alpha}(t, t') \right\}
\]

\[
\int_0^{t'} dt \left[ \sigma_{nm}^{\alpha}(t') K_{\alpha}(t', t) - \sigma_{mn}^{\alpha}(t') K_{\alpha}(t', t) \right] + (\sigma_{nm}^{\alpha} - \sigma_{mn}^{\alpha})(t) \int_0^{t'} dt K_{\alpha}(t', t) \right\}.
\]

We notice that

\[
[F_{mn}^{(i)}(t, t')] = F_{mn}^{(i)}(t', t),
\]

\[
[K_{mn}^{(i)}(t, t')] = K_{mn}^{(i)}(t', t),
\]

\[
[U_{mn}^{(i)}(t, t')] = \hat{V}_{mn}^{(i)}(t, t'),
\]

\[
[V_{mn}^{(i)}(t, t')] = \hat{U}_{mn}^{(i)}(t, t').
\]

D.4. Correlators and dissipative functions

The correlation function of the bath (D13) and the functional (D10) can be rewritten in terms of the dissipative functions defined by equation (37). Taking into account integrals, such as

\[
\int_0^{t'} dt \int_0^{t'} dt_1 K_{\alpha}(t_1, t_2) = f_\alpha(t) + f_\alpha^*(t') - f_\alpha(t - t'),
\]

we find that

\[
ln F_{mn}^{(i)}(t, t') = \sum_\alpha (\sigma_{mn}^{\alpha} - \sigma_{mn}^{\alpha})(\sigma_{mn}^{\alpha} - \sigma_{mn}^{\alpha}) f_\alpha(t - t')
\]

\[
- i \sum_\alpha \varepsilon_\alpha \left[ (\sigma_{mn}^{\alpha})^2 - (\sigma_{mn}^{\alpha})^2 \right] t - i \sum_\alpha \varepsilon_\alpha \left[ (\sigma_{mn}^{\alpha})^2 - (\sigma_{mn}^{\alpha})^2 \right] t'
\]

\[
+ \sum_\alpha (\sigma_{mn}^{\alpha} - \sigma_{mn}^{\alpha})(\sigma_{mn}^{\alpha} - \sigma_{mn}^{\alpha}) f_\alpha(t)
\]

\[
- \sum_\alpha (\sigma_{mn}^{\alpha} - \sigma_{mn}^{\alpha})(\sigma_{mn}^{\alpha} + \sigma_{mn}^{\alpha}) f_\alpha(t')
\]

\[
+ \sum_\alpha (\sigma_{mn}^{\alpha} - \sigma_{mn}^{\alpha})(\sigma_{mn}^{\alpha} f_\alpha(t) - \sum_\alpha (\sigma_{mn}^{\alpha} - \sigma_{mn}^{\alpha}) f_\alpha(t).
\]

Here the matrix elements \( \sigma_{mn}^{\alpha} \) and \( \sigma_{mn}^{\alpha} \) are taken at time \( t \), whereas the elements \( \sigma_{mn}^{\alpha} \) and \( \sigma_{mn}^{\alpha} \) depend on the time \( t' \).

The total reorganization energy \( \varepsilon_\alpha \) is defined by equation (38).

With equation (D16) we can calculate the correlator \( \langle S_{mn}(t) S_{mn}(t) \rangle \). It follows from equations (57) and (D4) that this correlator is determined by equations (D6) and (D10) where we have to put \( t' = 0 \):
\[ \langle S_{mn}^0(t) S_n(t) \rangle = F_{mn}^{m'n'}(t, t') = \exp \left[ - \sum_\alpha (\sigma_\alpha^m - \sigma_\alpha^n)^2 f_\alpha^m (t) \right] \mathbf{e}^{i \theta_{nm}(t)}, \] (D17)

with the phase

\[ \theta_{nm}(t) = \sum_\alpha \left[ (\sigma_\alpha^m)^2 - (\sigma_\alpha^n)^2 \right] [ f_\alpha^m (t) - \varepsilon_\alpha t]. \] (D18)

Taking into account equations (43) and (C1) we find that

\[ \langle S_{mn}^0(t) S_n(t) \rangle = e^{-\frac{\ln W_{mn}^2}{W_{mn}^2}} e^{i \theta_{nm}(t)} \left[ \sqrt{1 + \omega^2 t^2} \sinh(\pi T t) \right] \frac{\omega^m}{\pi T}. \] (D19)

Low-frequency, \( W_{mn}^2 = \alpha_{mn} W_2^2 \), and high-frequency, \( \alpha_{mn} = \alpha_{mn} W_1 \), parameters are proportional to the Hamming distance \( \alpha_{mn} \) between states \( |m\rangle \) and \( |n\rangle \) (49). At \( \alpha_{mn} \neq 0 \) the function \( \langle S_{mn}^0(t) S_n(t) \rangle \) rapidly decays within the time scale of \( 1/W_{mn} \). The average value of the operator (64) also does not survive during the annealing process since

\[ \langle \tilde{Q}_{mn}(t) \rangle \sim e^{i \theta_{nm}} \langle S_{mn}^0(t) S_n(t) \rangle \sim 0. \] (D20)

D.5. Selection rules

The real part of the exponent (D16) has the form

\[ \Re \{ \ln F_{mn}^{m'n'}(t, t') \} = \sum_\alpha (\sigma_\alpha^m - \sigma_\alpha^n)(\sigma_\alpha^{m'} - \sigma_\alpha^{n'}) f_\alpha^m (t - t') \]
\[ - \sum_\alpha \left[ (\sigma_\alpha^m)^2 - (\sigma_\alpha^n)^2 \right] \frac{f_\alpha^m (t) - f_\alpha^n (t')} {2} \]
\[ - \sum_\alpha (\sigma_\alpha^m - \sigma_\alpha^n + \sigma_\alpha^{m'} - \sigma_\alpha^{n'})^2 \frac{f_\alpha^m (t) + f_\alpha^n (t')} {2}. \] (D21)

We expect now that the time interval \( t - t' \) is short enough, so that \( t \sim t' \gg |t - t'| \). However, we have \( t \sim t_t \) and \( t' \sim t_t \), where \( t_t \) is the total annealing time. Notice also that the functions \( f_\alpha(t) \) and \( f_\alpha(t') \) are growing with time. It follows from the formulas in appendix C that the HF parts of the functions \( f_\alpha(t) \) and \( f_\alpha(t') \) are linearly increasing with time: \( f_\alpha(t) \sim \eta_T t \gg \frac{\delta}{\pi T} \gg \frac{1}{\omega} \). We assume that environments coupled to different qubits are described by the same dissipative functions as we do in section 3.5. The LF component \( f_\alpha(t) \) grows with time as well. This means that, during the annealing run, the contribution of the last line in equation (D21) suppresses the functional \( F_{mn}^{m'n'}(t, t') \) if the prefactor \( (\sigma_\alpha^m - \sigma_\alpha^n + \sigma_\alpha^{m'} - \sigma_\alpha^{n'})^2 \) is not equal to zero. The only surviving term in the matrix \( F_{mn}^{m'n'}(t, t') \) should have the set of indexes such that the relation

\[ \sigma_\alpha^m - \sigma_\alpha^n + \sigma_\alpha^{m'} - \sigma_\alpha^{n'} = 0 \] (D22)

is satisfied during the entire annealing process at \( t \sim t' \gg |t - t'| \). The relation (D22) is true at every annealing point for the indexes:

\[ m = n', \quad n = m'. \] (D23)

In this case, the real part of the exponent (D21) depends on the time interval \( t - t' \) only:

\[ \Re \{ \ln F_{mn}^{m'n'}(t, t') \} = - \sum_\alpha (\sigma_\alpha^m - \sigma_\alpha^n)^2 f_\alpha^m (t - t'). \] (D24)

We notice that the selection rules (D23) are derived provided that \( \sigma_\alpha^m = \langle m | \sigma_\alpha^z | m \rangle \neq 0 \) at some \( m \) and \( \alpha \).

At the condition (D23), we obtain the following expression for the functional \( F_{mn}(t, t') \equiv F_{mn}^{m'n'}(t, t') \),

\[ F_{mn}(t, t') = \exp \left\{ - \sum_\alpha (\sigma_\alpha^m - \sigma_\alpha^n)^2 f_\alpha^m (t - t') - i \sum_\alpha \varepsilon_\alpha \left[ (\sigma_\alpha^m)^2 - (\sigma_\alpha^n)^2 \right] (t - t') \right\} \]
\[ + 2i \sum_\alpha (\sigma_\alpha^m - \sigma_\alpha^n)^2 \sigma_\alpha^m \left[ f_\alpha^m (t) - f_\alpha^n (t') \right]. \] (D25)

With the selection rules (D23), the correlator (D13) takes the form

\[ \langle \tilde{Q}_{mn}(t) \tilde{Q}_{m'n'}(t') \rangle = \delta_{mn} \delta_{m'n'} \langle \tilde{Q}_{mn}(t) \tilde{Q}_{mn}(t') \rangle, \] (D26)
where
\[
\tilde{K}_{mn}(t, t') \equiv \langle \tilde{Q}_{mn}(t) \tilde{Q}_{nm}(t') \rangle = e^{i \int_0^{t'} d\tau \omega_{mn}(\tau)} \\
\times \left[ \sum_\alpha |\sigma_{mn}^\alpha|^2 K_\alpha(t, t') + U_{mn}(t, t') U_{nm}^\dagger(t', t) \right] F_{mn}(t, t').
\] (D27)

The function \( U_{mn}(t, t') \equiv U_{mn}^\dagger(t, t') \) is defined in equation (D14),
\[
U_{mn}(t, t') = \bar{T}_{mn} - \sum_\alpha \sigma_{mn}^\alpha (\sigma_m^\alpha - \sigma_n^\alpha) \tilde{g}_\alpha(t - t') - \sum_\alpha \sigma_{mn}^\dagger \sigma_m^\dagger \left[ \tilde{g}_\alpha(t) + \tilde{g}_\alpha(-t) \right].
\] (D30)

The function \( \tilde{g}_\alpha(t) \) is defined as: \( \tilde{g}_\alpha(t) = g_\alpha(t) - \varepsilon_\alpha \), where \( g_\alpha \) is shown in (37). We also notice that
\[
\tilde{g}_\alpha(t) + \tilde{g}_\alpha(-t) = -2 \int \frac{d\omega}{2\pi} \chi_\alpha^m(\omega) \frac{1 - \cos \omega t}{\omega}.
\] (D31)

Taking into account that the dissipative function \( g_\alpha(t) \) goes to zero at \( t \rightarrow \infty \), we obtain the steady-state expression for the function \( \tilde{U}_{mn}(t, t') \),
\[
\tilde{U}_{mn}(t, t') = \bar{T}_{mn} - \sum_\alpha \sigma_{mn}^\dagger \sigma_m^\dagger \varepsilon_\alpha.
\] (D33)

We presume that all matrix elements of qubit operators are taken at time \( t \).

For the case of qubits coupled to environments described in section 3.5, we obtain the following expression for the bath correlator (D27):
\[
\tilde{K}_{mn}(t, t') = e^{i \omega_{mn}(t') t} e^{-i \omega_{mn}(t) t'} e^{i(c_{\bar{\zeta}} - \bar{\zeta}) t} [b_{mn}(t') \tilde{f}(\tau) + [\bar{T}_{mn} - \varepsilon_{mn} \tilde{g}(\tau)] [\bar{T}_{mn}^\dagger - \varepsilon_{mn}^\dagger \tilde{g}^\dagger(\tau)]]
\] (D34)

where \( \tau = t - t' \). The parameter \( \zeta_{\alpha} \) has a meaning of a polaron shift [28, 29],
\[
\zeta_{\alpha} = \sum_\alpha \varepsilon_\alpha (\sigma_m^\alpha)^2.
\] (D35)

We notice that the polaron shift (D35) contains contributions of both, LF, \( \varepsilon_L \), and HF, \( \varepsilon_H \), parts of the bath reorganization energy since \( \varepsilon_{\alpha} = \varepsilon_L + \varepsilon_H \). The polaron shift introduced in equations (5) and (6) of [28] depends on LF noise only.

The bath correlator (D34) is characterized by a short correlation time \( \tau_{mn} \). The parameter \( \tau_{mn}^{-1} \) can be evaluated as
\[
\frac{1}{\tau_{mn}} = \max \{|E_m - E_n|, W_{mn}\}.
\] (D36)

**D.6. Cross-correlator** \( \langle \tilde{Q}_{mn}(t) \tilde{Q}_{kl}(t') \rangle \)

The cross-correlations are characterized by the function
\[
\langle \tilde{Q}_{mn}(t) \tilde{Q}_{kl}(t') \rangle = e^{i \phi_{mn}(t)} \sum_{\alpha'} \phi_k^{\alpha'}(t') \\
\times \int_0^{t'} d\tau' (S^k_{\alpha'}(t) [Q_{mn}(t) - \bar{T}_{mn}] S_{\alpha'}(t) \\
\times S^k_{\alpha'}(t', \tau)' Q_{kl}(\tau)' S_{\alpha'}(t', \tau')).
\] (D37)

Taking into account the definitions of the S-matrix (57) and (61) and applying the Wick theorem [45] for the Gaussian operators of the bath, we find that the correlator (D37) is proportional to the function \( \langle S^k_{\alpha'}(t) S_{\alpha'}(t) \rangle \).
given by equation (D17),

\[ \langle \hat{Q}_{mn}(t) \hat{Q}_{kl}(t') \rangle = J_{mn}^k(t, t') \times \langle S_{m}^l(t) S_n(t) \rangle, \tag{D38} \]

where

\[
J_{mn}^k(t, t') = i \mathcal{Z}_{mn}(t) e^{i\phi_{mn}(t')} \sum_{\alpha} \sigma_{mn}^\alpha(t') \times \int_0^{t'} d\tau \left\{ \sigma_{mn}^\alpha(t') \int_0^{\tau} d\tau' [K_n(\tau, \tau') - K_m(\tau, \tau')] + (\sigma_{mn}^\alpha - \sigma_{mn}^\alpha(t) \int_0^{t'} d\tau' K_m(\tau, \tau') \right\} \\
- e^{i\phi_{mn}(t')} \sum_{\alpha} \sigma_{mn}^\alpha(t) \sigma_{mn}^\alpha(t') \int_0^{t'} d\tau K_m(\tau, \tau), \tag{D39} \]

with the renormalized tunneling coefficient \( \mathcal{Z}_{mn}(t) \) defined as

\[
\mathcal{Z}_{mn}(t) = \tilde{t}_{mn} - i \sum_{\alpha} \sigma_{mn}^\alpha(t) \int_0^{t} dh [ \sigma_{mn}^\alpha(t) K_n(h) - \sigma_{mn}^\alpha(t) K_m(h, t)]. \tag{D40} \]

The most important fact here is that the cross-correlator (D38) is proportional to the function \( \langle S_{m}^l(t) S_n(t) \rangle \), which rapidly decays during the annealing process according to equation (D17). Therefore, the cross-correlators (D37) between diagonal and off-diagonal operators of the bath give no contribution to the evolution equation (78).

**Appendix E. Derivation of master equations**

The time evolution of the system operators \( \langle \Lambda_{mn} \rangle \) is governed by equation (78). We transform this relation to the set of master equations for the probabilities \( P_n \) defined by equation (74). To do that, we have to calculate products of bath and system operators, such as \( \langle Q_{mn}^l \Lambda_{kl} \rangle \), where \( \langle \ldots \rangle \) means averaging over free bath fluctuations. Operators \( \Lambda_{mn} \) and \( Q_{mn}^l \) are given by equations (73) and (76).

**E.1. Calculation of the correlator \( \langle Q_{mn}^l \Lambda_{kl} \rangle \)**

We begin by calculating a more general correlation function \( \langle Q_{mn}^l \Lambda_{kl} \rangle \) using a perturbation expansion up to the second order in the bath operators \( \hat{Q}_{mn} \) (64) and resorting to the methods outlined in [20, 31, 46]. It follows from equations (73) and (76) that

\[
\langle Q_{mn}^l(t) \Lambda_{kl}(t) \rangle = \langle U_l^*(t) \hat{Q}_{mn}(t) | k(t) \rangle \langle l(t) | U_l(t) \rangle, \tag{E1} \]

where the unitary matrix \( U_l \) (59) is determined by the Hamiltonian \( H_l \) given by equation (62). Using functional derivatives, up to the second order in operators \( \hat{Q}_{mn} \), we obtain

\[
\langle Q_{mn}^l(t) \Lambda_{kl}(t) \rangle = \langle U_l^*(t) \hat{Q}_{mn}(t) | k(t) \rangle \langle l(t) | U_l(t) \rangle \\
= \int dt' K_{mn}^{kl}(t, t') \left\{ \frac{\delta U_l^*(t)}{\delta Q_{mn}(t')} | k(t') \rangle \langle l(t') | U_l(t) \rangle + \int dt'' K_{mn}^{kl}(t, t') \left\{ U_l^*(t) | k(t') \rangle \langle l(t') | \frac{\delta U_l(t)}{\delta Q_{mn}(t')} \right\}, \right. \]

where \( K_{mn}^{kl} \) is the bath correlation function defined by equations (70), (71), and (D34). The cross-correlation functions, such as \( \langle \hat{Q}_{mn}(t) \hat{Q}_{mn'}(t') \rangle \), do not appear in the correlator \( \langle Q_{mn}^l \Lambda_{kl} \rangle \) since they do not survive the long annealing run. The average value of the bath operator \( \langle \hat{Q}_{mn}(t) \rangle \) also gives no contribution to equation (E1) as it follows from equations (D19) and (D20) obtained in appendix D.

We see from equation (59) that

\[
\frac{\delta U_l(t)}{\delta Q_{mn}(t)} = -iT \left\{ \int_0^{t'} d\tau \frac{\delta H_l(\tau)}{\delta Q_{mn}(t)} e^{-i \int_0^\tau d\tau' H_l(t)} \right\}. \]

With the Hamiltonian \( H_l \) given by equation (62), we find

\[
\frac{\delta H_l(\tau)}{\delta Q_{mn}(t)} = -\delta(t - \tau) | n'(t)\rangle \langle n'(t) |. \tag{E2} \]
For the functional derivatives of the unitary matrices $U_I$ and $U_I^\dagger$, we derive the relations:

$$\frac{\delta U_I(t)}{\delta Q_{m'n'}(t_I)} = i(\theta(t - t_I) U_{m'n'}(t_I)\Lambda_{m'n'}(t_I),$$

$$\frac{\delta U_I^\dagger(t)}{\delta Q_{m'n'}(t_I)} = -i(\theta(t - t_I) \Lambda_{m'n'}(t_I))U_I^\dagger(t).$$

(E3)

With these formulas in mind, we obtain the following expression for the correlator (E1):

$$\langle Q_{m'n}(t)\Lambda_{I}(t)\rangle = \int_0^t dt_1 \Lambda_{m'n'}(t_1)\Lambda_{m'n'}(t)\langle \Lambda_{I}(t_1)\rangle$$

$$-i\int_0^t dt_1 \Lambda_{m'n'}(t_1)\langle \Lambda_{I}(t_1)\rangle.$$

(E4)

In equation (78) we have terms such as $\langle Q_{m'n}^L(\Lambda_{mn})\rangle$. Using the selection rules (D26) we obtain

$$\langle Q_{m'n}(t)\Lambda_{mn}(t)\rangle = \int_0^t dt_1 \Lambda_{m'n'}(t_1)\langle \Lambda_{mn}(t_1)\rangle$$

$$-i\int_0^t dt_1 \Lambda_{m'n'}(t_1)\langle \Lambda_{mn}(t_1)\rangle.$$

(E5)

After the first step, the evolution equation (78) turns into the form

$$\frac{d}{dt}\langle \Lambda_{mn}(t)\rangle = \sum_{m=\alpha}^n \int_0^t dt_1 \Phi_{m'n'}(t, t_1)\langle \Lambda_{mn}(t)\Lambda_{mn}(t_1)\rangle$$

$$-\sum_{m=\alpha}^n \int_0^t dt_1 \Phi_{m'n'}(t, t_1)\langle \Lambda_{mn}(t_1)\Lambda_{mn}(t)\rangle + \{h.c.\},$$

(E6)

where $\{h.c.\}$ is the Hermitian conjugate of the previous terms. It is of interest that the time evolution of the system operator $\langle \Lambda_{mn}(t)\rangle$ depends on the behavior of the correlators, such as $\langle \Lambda_{mn}(t)\Lambda_{mn}(t')\rangle$.

**E.2. Correlator $\langle \Lambda_{mn}(t)\Lambda_{mn}(t')\rangle$**

As the next step in the derivation of master equations, we calculate the correlator of system operators in the right-hand side of equation (E6). Of interest is when the moments of time $t$ and $t'$ are separated by the short time interval $\tau_{mn}$ such that

$$t - t' \sim \tau_{mn} \ll t.$$

For equation (E6) the parameter $\tau_{mn}$ corresponds to the correlation time given by (D36). It follows from (75) that the evolution of the operator $\Lambda_{mn}$ is quite slow. The rate of this evolution is determined by the bath operators, such as $Q_{00}$ and $Q_{11}$, which are proportional to the off-diagonal elements of qubit Pauli matrices $\sigma^z_{lm}$ and $\sigma^z_{lk}$, and also to the off-diagonal terms such as $T_{mn}$ and $T_{nk}$; see equations (46), (48), (64), (68) for definitions. At first glance, this fact allows us to ignore the variation of $\Lambda_{mn}(t')$ within the interval $\tau_{mn}$. In this case, the correlator of system operators can be easily calculated:

$$\langle \Lambda_{mn}(t)\Lambda_{mn}(t')\rangle \approx \langle \Lambda_{mn}(t)\Lambda_{mn}(t)\rangle = \langle U_I^\dagger|n\rangle \langle n|U_I \rangle = \langle \Lambda_{mn}(t)\rangle.$$  

(E7)

We notice, however, that the sum of the off-diagonal elements, such as

$$\sum_{k=\alpha}^n \sigma^z_{lk} \sigma^z_{kn} = 1 - (\sigma^z_{nn})^2,$$

(E8)

is not small, even though each of the components of this sum is small by itself. Therefore, the system correlators in (E6) should be calculated more precisely.

To do this, we notice that the correlators in question satisfy the equation

$$i\frac{d}{dt}\langle \Lambda_{mn}(t)\Lambda_{mn}(t')\rangle = \sum_k \langle Q_{mk}^L(t)\Lambda_{kn}(t)\Lambda_{mn}(t')\rangle - \sum_k \langle Q_{kn}^L(t)\Lambda_{mk}(t)\Lambda_{mn}(t')\rangle,$$

(E9)

which follows from (75). We show that Markovian fluctuations of the bath characterized by zero-frequency susceptibility $\chi_{s,0}(t)$ contribute to the right-hand side of equation (E9). This contribution is significant because it is proportional to the sums $\sum_{k=\alpha}^n |\sigma^z_{nk}|^2$ given by equation (E8). We choose the system basis where the off-diagonal elements, such as $\sigma^z_{nk}$, are small, whereas the diagonal elements $\sigma^z_{nn}$ can take any values from the interval $[-1, 1]$. The components of the Pauli matrix $\sigma^z_{mn}$ are defined by equation (48). Notice that the Markovian contribution to the right-hand side of equation (E9) can be traced without resorting to the perturbation theory in the system–bath interaction. In the process, we drop perturbative terms, which are proportional to individual matrix elements of the Pauli matrices and also to the off-diagonal elements $\Phi_{mn}$ of the system Hamiltonian $H_S$.

For this reason, in the bath operators $Q_{mn}$ involved in (E9) and defined by equation (76), we assume that...
The first term in the right-hand side of equation (E9),
\[ \langle Q_{m}^{t}(t) \rangle \Lambda_{mk}(t) \Lambda_{nm}(t') = \sum_{\alpha} \sigma_{\alpha}^{m} e^{i \omega_{\alpha} \tau} \Xi_{mn}(t, t'), \]
is proportional to the factor
\[ \Xi_{mn}(t, t') = \langle U_{j}^{\dagger}(t) S_{n}^{\dagger}(t) Q_{n}(t) S_{m}(t) \rangle \langle t | U_{j}(t) \Lambda_{mn}(t') \rangle. \]  

(E10) From here on, matrix elements, such as \( \sigma_{\alpha}^{mn} \), and system operators, such as \( |\rangle \langle n| \), are taken at time \( t \). According to the Wick theorem [45], in equation (E10) we pair the Gaussian bath operator \( Q_{n}(t) \) with the other operators, which contain bath variables. Notice that, as follows from the definition in (37), pairings of \( Q_{n}(t) \) in (E10) with the matrices \( S_{n}^{\dagger}(t) \) and \( S_{m}(t) \) give rise to diagonal matrix elements, such as \( \sigma_{\alpha}^{n} \) and \( \sigma_{\alpha}^{m} \), and, therefore, to products such as \( \sigma_{\alpha}^{nm} \). These products do not combine into sums similar to (E8). Therefore, this kind of pairing should be omitted. The system operator \( \Lambda_{mn}(t') \) also contains free bath operators such as \( Q_{n}(t'') \) where \( t'' < t' < t \). The relation \( t' < t \) means that \( \Lambda_{mn}(t') \) cannot depend on the Markovian operator \( Q_{n}(t) \) taken at the future moment of time \( t \). For this reason, we do not consider pairings between \( Q_{n}(t) \) and \( \Lambda_{mn}(t') \) in (E10).

Taking pairings of \( Q_{n} \) and the operators \( U_{j}^{\dagger} \) and \( U_{j} \), we obtain
\[ \Xi_{mn}(t, t') = \int dt K_{n}(t, t) \left\{ \delta U_{j}^{\dagger}(t) \right\} \delta Q_{n}(t) \right\} \langle t | U_{j}(t) \Lambda_{mn}(t') \rangle, \]

where \( K_{n}(t, t) = \langle Q_{n}(t) Q_{n}(t) \rangle \) is the correlation function of the free bath. The matrices \( S_{n}^{\dagger} \) and \( S_{m} \) are taken at time \( t \). For the functional derivative of the matrix \( U_{j} \), we obtain
\[ \frac{\delta U_{j}(t)}{\delta Q_{n}(t)} = -i T \left\{ \int_{0}^{t} d\tau \frac{\delta H(t)}{\delta Q_{n}(t)} e^{-i \int_{0}^{t} dt_{j} \Lambda(t)} \right\}. \]

(E11) In the Hamiltonian \( H(t) \) we keep the component that is proportional to the free bath operator \( Q_{n}(t) \),
\[ H(t) = -\sum_{\alpha} \sum_{k' \neq k'} \sigma_{\alpha}^{k'k} e^{i \omega_{\alpha} \tau} S_{k'}^{\dagger}(t) Q_{n}(t) S_{k}(t) |k' \rangle \langle l' |. \]
The dominant term in the functional derivative of the Hamiltonian \( H \) has the form
\[ \frac{\delta H(t)}{\delta Q_{n}(t)} = -\delta(t - t) \sum_{k' \neq k} \sigma_{\alpha}^{k'k} e^{i \omega_{\alpha} \tau} S_{k'}^{\dagger}(t) S_{k}(t) |k' \rangle \langle l' |. \]

For the derivative (E12), we obtain
\[ \frac{\delta U_{j}(t)}{\delta Q_{n}(t)} = i \theta(t - t) \sum_{k' \neq k} \sigma_{\alpha}^{k'k} e^{i \omega_{\alpha} \tau} U_{j}(t) S_{k'}^{\dagger}(t) \Lambda_{k'}(t), \]

where we introduce the new bath operator
\[ S_{k}(t) = U_{j}^{\dagger}(t) S_{k'}^{\dagger}(t) S_{k}(t) U_{j}(t). \]

(E16) We also have the following formula
\[ \frac{\delta U_{j}^{\dagger}(t)}{\delta Q_{n}(t)} = -i \theta(t - t) \sum_{k' \neq k} \sigma_{\alpha}^{k'k} e^{i \omega_{\alpha} \tau} \Lambda_{k'}(t) S_{k'}^{\dagger}(t) U_{j}^{\dagger}(t). \]

(E17) With equations (E15) and (E17), the function \( \Xi_{mn}(t, t') \) (E11) takes the form
\[ \Xi_{mn}(t, t') = i \sum_{k' \neq k} \int_{0}^{t} dt K_{n}(t, t) \sigma_{\alpha}^{k'k} e^{i \omega_{\alpha} \tau} \times \langle \Lambda_{k}(t) S_{m}(t) \Lambda_{m}(t') \rangle - i \sum_{k' \neq k} \int_{0}^{t} dt K_{n}(t, t) \sigma_{\alpha}^{k'k} e^{i \omega_{\alpha} \tau} \times \langle \Lambda_{k'}(t) S_{m}(t) \Lambda_{m}(t') \rangle. \]

(E18) The bath correlator \( K_{n}(t, t) = K_{n}(t - t) \) is defined by equation (34). The Markovian part of this correlator has a sharp peak at \( t = t_{1} \). Its contribution to the function \( \Xi_{mn}(t, t') \) is described by equation (E18) where in all functions of \( t_{1} \) we have to put \( t_{1} = t \) and, after that, remove these functions from the integrals over time. We notice that operators \( \Lambda_{k}(t) \) (73) and \( S_{k'}^{\dagger}(t) \) (E16) taken at the same moment of time commute at any sets of
indexes. This fact allows us to calculate the same-time products of the system operators with relations outlined in (E7). In particular, we have
\[ \Lambda_{\alpha\beta}(t)\Lambda_{\gamma\delta}(t) = \delta_{\alpha\gamma}\Lambda_{\beta\delta}(t), \]
\[ \Lambda_{\alpha\beta}(t)\Lambda_{\delta\gamma}(t) = \delta_{\alpha\delta}\Lambda_{\beta\gamma}(t). \]

The function (E18) now turns to the form
\[ \Xi_{mn}^\alpha(t, t') = \int_0^t dt_1 K_{\alpha\beta}(t, t_1) \sum_{i=n}^m \sigma_{\alpha\beta}^i(t) e^{i\omega_{\alpha\beta} t_1} \langle S_{lm}(t_1)S_{lm}(t) \Lambda_{\alpha\beta}(t)\Lambda_{\alpha\beta}(t') \rangle \]
\[ - i \int_0^t dt_1 K_{\alpha\beta}(t, t_1) \sum_{i=k}^m \sigma_{\alpha\beta}^i(t) e^{i\omega_{\alpha\beta} t_1} \langle S_{lm}(t_1)S_{lm}(t) \Lambda_{\alpha\beta}(t)\Lambda_{\alpha\beta}(t') \rangle. \]  
(E19)

This function appears in (E.2) and, after that, in equation (E9) for the correlator \( \langle \Lambda_{mn}(t)\Lambda_{nm}(t') \rangle \). The secular part of \( \Xi_{mn}^\alpha(t, t') \) should contain the correlator of system operators with the same set of indexes. In the first term in the right-hand side of equation (E19) we have to put \( k = m \) and \( l = n \), which is impossible since \( l \neq n \). Therefore, the first component of \( \Xi_{mn}^\alpha(t, t') \) has no secular term. In the second part of (E19) we take that \( l = m \).

This is accepted if \( m = k \). Thus, the secular part of the function \( \Xi_{mn}^\alpha(t, t') \) can be written as
\[ \Xi_{mn}^\alpha(t, t') = -i \int_0^t dt_1 K_{\alpha\beta}(t, t_1) \sigma_{\alpha\beta}^m(t) e^{i\omega_{\alpha\beta} t_1} \langle \Lambda_{mn}(t)\Lambda_{nm}(t') \rangle. \]  
(E20)

Here we take into account that \( S_{mn}(t)S_{nm}(t) = 1 \). The secular part of (E.2) has the form
\[ \langle Q_{\alpha\beta}(t)\Lambda_{mn}(t)\Lambda_{nm}(t') \rangle = -i \langle \Lambda_{mn}(t)\Lambda_{nm}(t') \rangle \sum_\alpha |\sigma_{\alpha\beta}^m(t)|^2 \int_0^t dt_1 K_{\alpha\beta}(t, t_1). \]  
(E21)

With the same approach, we obtain a secular component of the last term in (E9):
\[ \langle Q_{\alpha\beta}(t)\Lambda_{mn}(t)\Lambda_{nm}(t') \rangle = i \langle \Lambda_{mn}(t)\Lambda_{nm}(t') \rangle \sum_\alpha |\sigma_{\alpha\beta}^m(t)|^2 \int_0^t dt_1 K_{\alpha\beta}(t, t_1). \]  
(E22)

We notice that nonscalar terms in the right-hand side of equation (E9) are proportional to the products of \( S \) matrices of the bath, such as given by equation (D19). These terms rapidly disappear over time.

The correlator of Markovian fluctuations of the bath to the evolution of the correlator of system operators is described by the following equation:
\[ \frac{d}{dt} \langle \Lambda_{mn}(t)\Lambda_{nm}(t') \rangle = -\sum_{k=n}^m |\sigma_{mn}^k(t)|^2 \int_0^t dt_1 K_{\alpha\beta}(t, t_1) \langle \Lambda_{mn}(t)\Lambda_{nm}(t') \rangle + \sum_{k=n}^m \sum_{m=k}^m |\sigma_{mk}^\alpha(t)|^2 \int_0^t dt_1 K_{\alpha\beta}(t, t_1) \langle \Lambda_{mn}(t)\Lambda_{nm}(t') \rangle. \]  
(E23)

The correlator \( K_{\alpha\beta}(t) \) of the free bath is defined in section 3.4 together with a susceptibility \( \chi_{\alpha\beta}(\omega) \) and the spectrum \( S_0(\omega) \). The upper limit \( t \) in (E23) can be replaced by infinity since the annealing time scale \( r \) is much longer than the correlation time of the bath. Taking into account the fluctuation-dissipation theorem (41) and the fact that \( \chi_{\alpha\beta}(0) = 2\epsilon_{\alpha\beta} \), we obtain
\[ \int_0^\infty dt K_{\alpha\beta}(t, t_1) = T\gamma_{\alpha\beta} - i\epsilon_{\alpha\beta}, \]  
(E24)

where
\[ \gamma_\alpha = \frac{\chi_\alpha'(\omega)}{\omega} \bigg|_{\omega=0} \]

is a negligibly small parameter, \( \gamma_{\alpha\beta} = \gamma_{\beta\alpha} = \eta/2 \). Finally, keeping the main contributions to (E9), we derive a simple equation which governs the short-time evolution of the system correlator:
\[ \frac{d}{dt} \langle \Lambda_{mn}(t)\Lambda_{nm}(t') \rangle = i \sum_\alpha \epsilon_{\alpha\beta} \left( \sum_{k=n}^m |\sigma_{mn}^k(t)|^2 - \sum_{m=k}^m |\sigma_{mk}^\alpha(t)|^2 \right) \langle \Lambda_{mn}(t)\Lambda_{nm}(t') \rangle. \]  
(E25)

The solution of this equation,
\[ \langle \Lambda_{mn}(t)\Lambda_{nm}(t') \rangle = e^{i\zeta_m(t-t')} \langle \Lambda_{mn}(t') \rangle, \]  
(E26)

has the additional factor oscillating in time with the frequency \( \zeta_m - \zeta_n \). Here we take into account equation (E8) and also the definition (D35) of the polaron shift \( \zeta_m \).

\textbf{E.3. Equations for system operators (}\lambda_{mn}\textbf{)}

As the next step, we substitute the correlation functions (E26) to equation (E6) taking into account that \( t' = t \). In the process, the system operator \( \langle \Lambda_{mn}(t) \rangle \) is replaced by \( \langle \Lambda_{mn}(t) \rangle \) since this variable is practically unchanged.
during the correlation time $\tau_{nm}$ of the function $e^{iw_n \tau} \hat{K}_{nm}(\tau)$, where $\tau = t - t_n$. Equation (E6) transforms to the equation for the system operator $\langle \Lambda_{nm} \rangle$,

$$\langle \Lambda_{nm} \rangle + \Gamma_n \langle \Lambda_{nm} \rangle = \sum_m \Gamma_{nm} \langle \Lambda_{nm} \rangle,$$

(E27)

with the relaxation matrix $\Gamma_{nm}$

$$\Gamma_{nm} = \int_0^\infty d\tau \hat{K}_{nm}(\tau) e^{i(w_n - w_m)\tau} + \{\text{h.c.}\},$$

(E28)

and with the rate $\Gamma_n = \sum_m \Gamma_{nm}$. Notice that $\hat{K}_{nm}(\tau) = \hat{K}_{nm}(-\tau)$, and that the matrix $\Gamma_{nm}$ has no diagonal elements. The matrix elements of the qubit operators involved in equation (E28) are taken at time $t$. The bath correlator $\hat{K}_{nm}(\tau)$ is given by equation (D27), and also by the simpler expression (D34). Taking these formulas into account, we derive equation (80) for the relaxation matrix $\Gamma_{nm}$. It is of interest that the polaron shifts in equation (E28) precisely cancel the polaron shifts in the bath correlator (D34) so that the rate (80) does not contain $\zeta_n$ and $\zeta_m$. This is especially important for the multiqubit system where the relative shift of two levels, $\zeta_m - \zeta_n$, can be quite large. The master equation (79) for the probability distribution of the system over basis states follows from equation (E27) if we apply the procedure (74) that turns the system operator $\langle \Lambda_{nm} \rangle$ into the probability $P_n$.

E.4. Equations for system operators $\langle \Lambda_{nm} \rangle$

The time evolution of the qubit operator $\langle \Lambda_{nm} \rangle$, where $m \neq n$, can be found from equation (75) averaged over free bath fluctuations. Using the results of the previous subsection, and also a secular approximation, we obtain the simple equation for the function $\langle \Lambda_{nm} \rangle$,

$$\langle \Lambda_{nm} \rangle + \left( \Gamma_n + \frac{\Gamma_m}{2} + i \frac{\delta_n - \delta_m}{2} \right) \langle \Lambda_{nm} \rangle = 0.$$

(E29)

Here, as in the previous subsection, the line width of the $n$-level is defined as $\Gamma_n = \sum_k \Gamma_{kn}$, where the rates $\Gamma_{kn}$ are determined by equation (E28). These rates are given by equation (82) for the case of identical environments, with the spectra $S_n(\omega) = S(\omega)$. In the more general case different qubits are coupled to different environments, and these environments have different spectral functions, such as $S_n(\omega) \neq S(\omega)$ at $\alpha \neq \beta$. In this case the rate $\Gamma_{nm}$ can be expressed in terms of the function $G_{nm}(\omega)$:

$$\Gamma_{nm} = G_{nm}(\omega_{nm}),$$

(E30)

where

$$G_{nm}(\omega) = \int_{-\infty}^{\infty} d\tau e^{i\omega \tau} e^{-\sum_\alpha [\sigma_n^\alpha - \sigma_m^\alpha] f_{\alpha}(\tau)}$$

$$\times \left\{ \sum_\alpha [\sigma_n^\alpha f_{\alpha}^*(\tau) + \left[ T_{mn} - \sum_\alpha \sigma_n^\alpha (\sigma_m^\alpha - \sigma_n^\alpha) g_{\alpha}(\tau) \right] T_{mn}^* - \sum_\alpha \sigma_n^\alpha (\sigma_m^\alpha - \sigma_n^\alpha) g_{\alpha}(\tau) \right\}. $$

(E31)

The renormalized matrix element $T_{mn}$ is given by equation (D33). In accordance with the dispersion relations, the frequency shift $\delta_n$ is also defined in terms of the function $G(\omega)$,

$$\delta_n = -\sum_k \int d\omega \frac{G_{kn}(\omega)}{\pi} \omega_{nm},$$

(E32)

Here, there is no simple convolution form for the function $G_{nm}(\omega)$ and for the rate $\Gamma_{nm}$, as it takes place for the case of identical environments described in section 5. We notice that equation (E30) is equivalent to equation (E28) from the previous subsection.

Appendix F. Gaussian and Lorentzian line shapes

In this appendix we describe properties of the functions $G_{nm}^L(\omega)$ and $G_{nm}^H(\omega)$ used in section 5.1. The LF envelope (with an index $\mu = L$) and the HF function (with $\mu = H$) are defined as

$$G_{nm}^\mu(\omega) = \int_{-\infty}^{\infty} d\tau e^{i\omega \tau} e^{-\alpha_{nm} f_{\mu}(\tau)}.$$  

(F1)

The LF dissipative function $f_L$ is given by equation (43). The function $G_{nm}^L(\omega)$ is described by a Gaussian lineshape,
G^L_{mn}(\omega) = \int \! d\tau \ e^{i(\omega-\omega_{mn})\tau - W^2_{mn}/2} = \frac{2\pi}{W^2_{mn}} \exp \left\{ -\frac{(\omega - \omega_{mn})^2}{2W^2_{mn}} \right\}, \quad (F2)

where \( \omega_{mn} = a_{mn} \omega_{fl} \) and \( W^2_{mn} = a_{mn} W^2 = 2 \sigma_{mn} T. \) At \( \omega_{mn} \to 0, \) we have \( G^L_{mn}(\omega) \to 2\pi\delta(\omega). \)

We assume that the HF function \( G^H_{mn}(\omega), \) defined by equation (F1) where \( \mu = H, \) includes the case of strong interaction of qubits with a Markovian heat bath. This bath is characterized by the flat spectrum \( S_f(\omega) = S_f(0) \) and by the function \( f_f(\tau) = \frac{1}{2} S_f(0)\tau^2. \) The function \( G^H_{mn}(\omega) \) related to the Markovian bath has a Lorentzian shape [25],

\[
G^H_{mn}(\omega) = \frac{2\gamma_{mn}}{\omega^2 + \gamma^2_{mn}},
\]

(F3)

In the Markovian case the linewidth \( \gamma_{mn} \)

\[
\gamma_{mn} = \frac{a_{mn}}{2} S_f(0),
\]

should be much smaller than the inverse correlation time of the HF bath. We also expect that the function \( G^H_{mn}(\omega) \) covers a weak interaction of qubits with a non-Markovian bath characterized by the frequency-dependent spectrum \( S_f(\omega). \) Taking into account that in the weak-coupling limit the function \( f_f \) is small, we expand the exponent in equation (F1) and keep linear terms in power of \( f_f. \) We obtain the following formula for the function \( G^H_{mn}(\omega): \)

\[
G^H_{mn}(\omega) = 2\pi\delta(\omega) \left[ 1 - a_{mn} \int \frac{dx}{2\pi} \frac{S_f(x)}{x^2} \right] + a_{mn} S_f(\omega) / \omega^2.
\]

(F5)

Equations (F3) and (F5) can be combined by a straightforward modification of the Markovian expression (F3),

\[
G^H_{mn}(\omega) = \frac{a_{mn}}{2} \frac{S_f(\omega)}{\omega^2 + \gamma^2_{mn}}.
\]

(F6)

Evidently, at \( S_f(\omega) = S_f(0), \) equation (F6) includes the Markovian case (F3). In the limit of zero qubit-bath coupling (at \( S_f(0) \to 0 \)) both expressions, (F5) and (F6), turn into \( \delta(\omega) \) function, \( G^H_{mn}(\omega) \to 2\pi\delta(\omega). \) Finally, at nonzero frequencies, \( \omega \gg \gamma_{mn} \) both functions, (F5) and (F6), are inversely proportional to the frequency squared and linearly proportional to the noise spectrum \( S_f(\omega), \) as it takes place in the Bloch–Redfield limit: \( G^H_{mn}(\omega) = a_{mn} S_f(\omega) / \omega^2. \) This means that the Lorentzian line shape (F6) provides an appropriate description of the function \( G^H_{mn}(\omega) \) in the whole range of frequencies.

Both functions, \( G^H_{mn}(\omega) \) (F2) and \( G^H_{mn}(\omega) \) (F6), meet the equilibrium condition,

\[
\frac{G^H_{mn}(\omega)}{G^H_{mn}(-\omega)} = e^{i\omega T},
\]

(F7)

and the normalization condition,

\[
\int \frac{d\omega}{2\pi} G^H_{mn}(\omega) = 1.
\]

(F8)

The normalization condition directly follows from the definition (F1). We recall that the index \( \mu \) takes two values: \( \mu = L, H. \)

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