Unified Theory of Dynamically Suppressed Qubit Decoherence in Thermal Baths

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We develop a unified theory of dynamically suppressed decay and decoherence by external fields in qubits coupled to arbitrary thermal baths and dephasing sources. This general theory does not invoke the rotating-wave approximation, which fails for ultrafast field-induced modulations of qubit-bath coupling. Considerations for optimizing the dynamical suppression are outlined.

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The suppression of quantum-state decay and decoherence in qubits interacting with their environment is the coveted key to quantum-information (QI) processing. To this end, a variety of methods have been proposed: (i) quantum error-correction and error-prevention codes [1], requiring ancillary qubits; (ii) decoherence-free subspace approaches [2], which exploit symmetry properties of qubit-environment interactions; and (iii) dynamical control of qubit-environment interactions by external fields [3–5]. The spectra of baths (continua) corresponding to vibrational or collisional decay or decoherence typically have limited widths ($\lesssim 10^{13}$ s^{-1}), and hence may allow *dynamical suppression* using feasible rates of modulation [3,4]. These results hold the promise that modulation of qubit-bath coupling may be very useful for QI processing. However, there is still no general theory of a qubit whose coupling to a finite-temperature bath or a dephasing source is modulated by an *arbitrary* time-dependent field. Here we present such a theory, addressing several basic questions: (a) Would *the qubit model hold* at all for *ultrafast modulation* rates that are comparable to its transition frequency ω_a (between its states $|e\rangle$ and $|g\rangle$), although such rates may invalidate the standard rotating-wave approximation (RWA) [6]? (b) Would *temperature effects*, which are known to incur *upward* $|g\rangle \to |e\rangle$ transitions [7], further complicate the dynamics and perhaps hinder the suppression of decay? (c) How to control both decay [3,4] and proper dephasing [5] in an efficient, *optimal* fashion that is compatible with quantum *gate operations?*

We explicitly consider a driven two-level system (TLS) undergoing decay into a finite-temperature bath, as well as proper dephasing, while its resonant frequency and *dipolar* coupling to the bath are dynamically modulated by external fields. The total Hamiltonian is $H = H_S(t) + H_B + H_I(t)$, where S, B, and I label the system, bath, and their interaction, respectively. These terms consist of

$$
\begin{gathered}
H_S(t) = \hbar[\omega_a + \delta_a(t) + \delta_r(t)]|e\rangle\langle e| + V(t)\sigma_x, \\
H_B = \sum_\lambda \hbar\omega_\lambda a_\lambda^\dagger a_\lambda, \qquad H_I(t) = \hbar S(t) B, \\
S(t) = \tilde{\epsilon}(t)\sigma_x, \qquad B = \sum_\lambda (\kappa_\lambda a_\lambda + \kappa_\lambda^* a_\lambda^\dagger).
\end{gathered}
\tag{1}
$$

In $H_S(t)$, $\delta_a(t)$ is the dynamically imposed ac Stark shift of the TLS resonance frequency ω_a and $\delta_r(t)$ is its *random* counterpart representing *proper dephasing*. The control (flipping) field $V(t) = V_0(t)e^{-i\omega_c t}$ + c.c., $V_0(t)$ being the Rabi frequency, couples to $\sigma_x = |e\rangle\langle g| + |g\rangle\langle e|$, the dipole-transition operator. The bath oscillator modes λ in H_B are described by the frequency ω_λ and annihilation operator a_λ. The time-modulated system-bath interaction $H_I(t)$ is affected by the dipolar operator $S(t) = \tilde{\epsilon}(t)\sigma_x$, with the *real* amplitude $\tilde{\epsilon}(t)$, and κ_λ is the coupling amplitude to mode λ. Clearly, terms such as $|e\rangle\langle g|\kappa_\lambda^* a_\lambda^\dagger$ or $|g\rangle\langle e|\kappa_\lambda a_\lambda$ in the system-bath interaction $H_I(t)$ are *antiresonant*. This general form of $H_I(t)$, unlike previous treatments [4], *does not invoke the RWA* [6], which may fail for ultrafast modulation.

Using Zwanzig's projection-operator technique to trace out the bath in Liouville's equation of motion [8], we have derived, from Eq. (1), a differential master equation (ME) for the density operator of the system $\rho(t)$, to *second order* in the system-bath coupling,

$$
\dot{\rho} = -\frac{i}{\hbar}[H_S(t), \rho] + \int_0^t dt' \{\Phi_T(t-t')[\tilde{S}(t',t)\rho, S(t)] + \text{H.c.}\}.
\tag{2}
$$

Here

$$
\Phi_T(t) = \langle \exp(iH_B t/\hbar) B \exp(-iH_B t/\hbar) B \rangle_B
\tag{3}
$$

is the "memory" or correlation function (CF) of the bath and $\langle \ldots \rangle_B = \mathrm{Tr}(\ldots \rho_B)$, where $\rho_B = Z^{-1}\exp(-\beta H_B/\hbar)$ is the density matrix of the bath in equilibrium, with Z as the normalization factor, and $\beta = \hbar/k_B T$ the inverse temperature (in time units). We have used in (2) the unitarily transformed dipole operator

$$
\begin{gathered}
\tilde{S}(t', t) = U_S(t, t') S(t') U_S^\dagger(t, t'), \\
U_S(t, t') = T_+ \exp\left[-\frac{i}{\hbar}\int_{t'}^t H_S(\tau) d\tau\right],
\end{gathered}
\tag{4}
$$

T_+ being the time-ordering operator. Equation (2) *generalizes* previously known non-Markovian MEs [6,8] to *arbitrary* time-dependent driving for the system and modulation of the system-bath coupling. By restricting our ME to second order in coupling (the Born approximation), we exclude the effects of changing the bath state in the course of its interaction with the system.

We then obtain our *generalized* Bloch equations for the components of $\rho(t)$:

$$\dot{\rho}_{ee} = -\dot{\rho}_{gg} = iV(t)(\rho_{eg} - \rho_{ge}) - R_e(t)\rho_{ee} + R_g(t)\rho_{gg}, \tag{5a}$$

$$\dot{\rho}_{eg} = \dot{\rho}^*_{ge} = -\{R(t) + i[\tilde{\omega}_a(t) + \delta_a(t) + \delta_r(t)]\}\rho_{eg} + iV(t)(\rho_{ee} - \rho_{gg}) + [R(t) - i\Delta_a(t)]\rho_{ge}. \tag{5b}$$

Equations (5) are more general than the previously investigated Bloch equations (compare with [6]) by virtue of their dynamically modified decay rates and spectral shifts. Thus, they account for *upward transitions* $|g\rangle \to |e\rangle$ [caused by either temperature or antiresonant, non-RWA, effects (see below)] at a rate $R_g(t)$, in addition to *downward* decay $|e\rangle \to |g\rangle$ at a rate $R_e(t)$. Their half-sum $R(t) = [R_e(t) + R_g(t)]/2$ contributes to the decoherence rate, which is further augmented by the random (proper-dephasing) shift $\delta_r(t)$ (see below). The resonance frequency is dynamically shifted by $\tilde{\omega}_a(t) - \omega_a = \Delta_a(t) = \Delta_e(t) - \Delta_g(t)$, where $\hbar\Delta_{e(g)}(t)$ is the Lamb shift of $|e\rangle$ ($|g\rangle$), caused by the dynamically modified coupling to the bath. The last term on the right-hand side of Eq. (5b) is known as "nonsecular" [6]; it is negligible, provided the modulated resonant frequency $\omega_a + \delta_a(t) \gg R(t) + |\Delta_a(t)|$.

The concurrent actions of the control field $V(t)$ (rotations around the x axis of the Bloch sphere) and the level modulation $\delta_a(t)$ (rotations around the z axis of the Bloch sphere) do not commute and thus complicate the dynamics. We shall therefore investigate Eqs. (5) separately during the *storage time,* when the control field is off [$V(t) = 0$], and during *gate operations,* when the modulating (off-resonant) field is off [$\delta_a(t) = 0$, $\tilde{\epsilon}(t) = 1$].

Consider first situations wherein $R(t)$, *the (dynamically modified) rate of bath-induced decoherence, is dominant compared to the proper-dephasing rate* [determined by $\delta_r(t)$], so that the latter may be neglected in Eq. (5b). The dynamically affected transition rates and shifts in (5) are then obtained from Eqs. (2) during the storage time, when $V = 0$, and found to be the real and imaginary parts of the expression

$$R_i(t)/2 + i\Delta_i(t) = \int_0^t dt' \Phi_T(t - t')K_i(t, t'),$$
$$K_i(t, t') = \langle i|S(t)\tilde{S}(t', t)|i\rangle \qquad (i = e, g), \tag{6}$$

written in terms of the bath CF $\Phi_T(t)$ [Eq. (3)] and the dipole CF $K_i(t, t')$. One can show that

$$K_e(t, t') = K_g^*(t, t') = \epsilon(t)\epsilon^*(t'),$$
$$\epsilon(t) = \tilde{\epsilon}(t)\exp\left[i\omega_a t + i\int_0^t \delta_a(\tau)d\tau\right], \tag{7}$$

where $\epsilon(t)$ is the dipole-modulation function, allowing for both amplitude and phase modulations. Hence, we have found how the decay and decoherence rates are determined by the convolution of the bath and dipole-coupling CFs.

We shall restrict Eqs. (6) and (7) to *coherent quasiperiodic modulation* of the dipolar coupling, $\epsilon(t) = \sum_k \epsilon_k e^{i\omega_k t}$, where ω_k ($k = 0, \pm 1, \dots$) are arbitrary discrete frequencies with the minimal spectral distance Ω. This is the most general quasistationary form of modulation. Without losing generality, we can assume that $\sum_k |\epsilon_k|^2 = 1$. The rates $R_{e(g)}(t)$ then tend to the long-time limits (their transient behavior has an insignificant effect, in view of the validity conditions stated in the next paragraph)

$$R_{e(g)} = 2\pi \int_{-\infty}^{\infty} d\omega F(\omega)G_T(\pm\omega) = 2\pi\sum_k |\epsilon_k|^2 G_T(\pm(\omega_a + \omega_k)), \tag{8}$$

where the upper (lower) sign corresponds to the subscript e (g), $F(\omega) = \sum_k |\epsilon_k|^2 \delta(\omega - \omega_a - \omega_k)$ is the spectral density (SD) of $K_e(t, t')$ [Eq. (7)] for quasiperiodic modulation, and the SD of the bath CF is

$$G_T(\omega) = (2\pi)^{-1} \int_{-\infty}^{\infty} \Phi_T(t)e^{i\omega t}dt = [n(\omega) + 1]G_0(\omega) + n(-\omega)G_0(-\omega). \tag{9}$$

Here the bath-coupling spectrum [7] at $T = 0$ is $G_0(\omega) = \sum_\lambda |\kappa_\lambda|^2 \delta(\omega - \omega_\lambda)$ and $n(\omega) = (e^{\beta\omega} - 1)^{-1}$ is the average number of quanta in the oscillator (bath mode) with frequency ω. Function (9) can be seen to be non-negative, with $G_T(-\omega) = e^{-\beta\omega}G_T(\omega)$, and vanish for $\omega < 0$ at $T = 0$: $G_0(\omega) = 0$ ($\omega < 0$) [see Fig. 1, inset (b)].

Equation (8) is the *pivotal general expression* derived in this Letter: it shows that R_e and R_g *are given by the overlap of the modulation spectrum $F(\omega)$ with the bath-CF spectra $G_T(\omega)$* and $G_T(-\omega)$, respectively. The limits (8) are approached when $\Omega t \gg 1$ and $t \gg t_c$. Here t_c is the bath-memory (correlation) time, defined as the largest inverse spectral interval over which $G_T(\omega)$ and $G_T(-\omega)$ change around the relevant frequencies $\omega_a + \omega_k$. The physical sense of Eq. (8) is that fast modulation of the system-bath coupling, at a frequency ω_k, drives the system out of resonance with the bath oscillations, thereby reducing the decay. The only criterion for the validity of (8) is that $R_{e(g)}t_c \ll 1$; i.e., the system decays much slower than the correlation (memory) time. Since both $R_{e(g)}$ and t_c depend on the modulation, this criterion may be achieved using a suitable modulation, even if in the absence of modulation the coupling is strong. Thus our ME indicates how to reduce decay and decoherence *irrespective of the strength of the coupling.*

We stress the universality of the result (8), by contrast to previous RWA treatments [4]. Had we used the standard

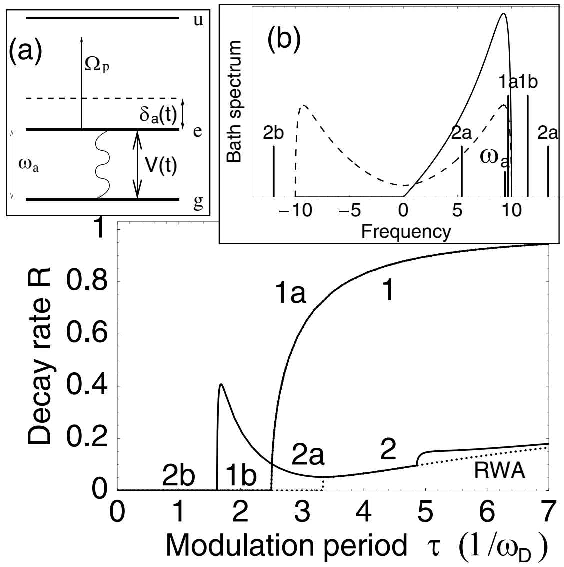

FIG. 1. Inset (a): Modulation scheme: a nonresonant field with Rabi frequency Ω_p Stark-shifts level e by $\delta_a(t)$, whereas $V(t)$ is the near-resonant (flipping) modulation of the $e-g$ transition. Inset (b): Overlap of bath and modulation spectra (arbitrary units): solid curve: $G_0(\omega)$; dashed curve: $G_S(\omega) = [G_T(\omega) + G_T(-\omega)]/2$ for 1D phonon bath (see text), $\beta = 10/\omega_D$; vertical bars: peaks of $F(\omega)$, located relative to $\omega_a = 0.94\omega_D$; bars 1*a* and 1*b*: $\phi = -0.15$, single peak for each choice of τ; bars 2*a* and 2*b*: $\phi = \pi$, pairs of peaks for each choice of τ. Lower figure: decay rates $R = (R_e + R_g)/2$ (normalized to the unperturbed R) as a function of the modulation period τ (in units of $1/\omega_D$) for the spectra shown in inset (b): curves 1*a* and 1*b* and curves 2*a* and 2*b* correspond to the peaks of $F(\omega)$ in inset (b); dotted curves: RWA calculations of curves 1 and 2. Curve 1 is optimal.

dipolar RWA Hamiltonian in the case of an oscillator bath, dropping the antiresonant terms in $H_I(t)$ [Eq. (1)], we would have arrived at the transition rates $R_{e(g)}^{\mathrm{RWA}} = 2\pi\int_0^\infty d\omega F(\omega)G_T(\pm\omega)$, wherein the integration is performed from 0 to ∞, rather than from $-\infty$ to ∞, as in (8). This means that the RWA transition rates hold for a slow modulation, when $F(\omega) \simeq 0$ at $\omega < 0$, being peaked near ω_a. However, whenever the suppression of $R_{e(g)}$ requires modulation at a rate comparable to ω_a, the RWA is inadequate. For instance, Eq. (9) implies that, at $T = 0$, the rate R_g^{RWA} vanishes identically, irrespective of $F(\omega)$, in contrast to the true upward-transition rate R_g in Eq. (8), which may be comparable to R_e for ultrafast modulation. The difference between the RWA and non-RWA decay rates stems from the fact that the RWA implies that a downward (upward) transition is accompanied by emission (absorption) of a bath quantum, whereas the non-RWA (negative-frequency) contribution to $R_{e(g)}$ in Eq. (8) allows for just the opposite: downward (upward) transitions that are accompanied by absorption (emission). The latter processes are possible since the modulation may cause *level* $|e\rangle$ *to be shifted below* $|g\rangle$.

The validity of the (decohering) qubit model during time t in the presence of modulation at an ultrafast rate exceeding ω_a is now elucidated: it requires that $R_{e(g)j}t \ll 1$, $R_{e(g)j}$ being the effective transition rate from level e (g) to *any other* level j, and, in particular, $R_{e(g)}t \ll 1$.

We shall now apply these general results to a qubit that undergoes decay via coupling to a phonon bath, which is modeled by the function [9] $G_0(\omega) = [A\omega\sqrt{\omega_D - \omega}/(\eta + \omega_D - \omega)]\theta(\omega_D - \omega)$. Here ω_D is the Debye (cutoff) frequency, η is the smoothing parameter, and $\theta()$ is the step function. The spectrum of $G_0(\omega)$ is that of a one-dimensional (1D) system, e.g., a linear multi-ion trap [1] for $\eta \to 0$, whereas for $\eta \neq 0$ it characterizes a 3D system, e.g., a solid matrix wherein *a qubit* is embedded. The function $G_0(\omega)$ and the symmetrized function $[G_T(\omega) + G_T(-\omega)]/2$ are shown in Fig. 1, inset (b), for a low-temperature $\beta = 10/\omega_D$. One observes that $G_T(\omega)$, unlike $G_0(\omega)$, is nonzero at $\omega < 0$ for $\beta < \infty$. Generally, $G_T(\omega)$ has two cutoffs, at $\omega = \pm\omega_D$. For high temperatures, $\beta \ll 1/\omega_D$, $G_T(\omega)$ tends to be even, $G_T(\omega) \simeq G_T(-\omega)$ [cf. Eq. (9)], whereas, for low temperatures, $\beta \gg 1/\omega_D$, the lower cutoff of $G_T(\omega)$ is effectively at $\omega < -1/\beta$.

In the absence of modulation, the decay rates (8) obey Fermi's golden rule: $F(\omega) \approx \delta(\omega - \omega_a)$, $R_{e(g)} \approx 2\pi G(\pm\omega_a)$. The upward rate R_g at the low-temperature $\beta = 10/\omega_D$ is then close to zero, and R_e dominates. The ultrafast quasiperiodic modulation may modify $R_{e(g)}$ according to (8) by shifting $G_T(\pm\omega_a) \to \sum_k |\epsilon_k|^2 G_T(\pm(\omega_a + \omega_k))$. *Optimization* requires the choice of $|\epsilon_k|^2$ so as to minimize Eq. (8) for the smallest ω_k possible.

We shall specifically consider *impulsive phase modulation (IPM),* consisting of phase jumps by an amount ϕ at times $\tau, 2\tau, \ldots$, which can be effected by a train of identical, equidistant, narrow pulses of nonresonant radiation. The long-time decay is then given by Eq. (8) with [3] $\omega_k = 2k\pi/\tau - \phi/\tau$ and $|\epsilon_k|^2 = 4\sin^2(\phi/2)/(2k\pi - \phi)^2$. For *small phase shifts,* $|\phi| \ll \pi$, the $k = 0$ peak dominates, $|\epsilon_0|^2 \simeq 1 - \phi^2/12$, whereas $|\epsilon_k|^2 \simeq \phi^2/4\pi^2k^2$ for $k \neq 0$. Then the modulation acts as a *constant frequency shift* $\Delta = -\phi/\tau$ of the response: $G_T(\pm\omega_a) \to G_T(\pm(\omega_a + \Delta))$. With the increase of $|\phi|$, the difference between the $k = 0$ and $k = 1$ peak heights diminishes, *vanishing* for $\phi = \pm\pi$. Then $|\epsilon_0|^2 = |\epsilon_1|^2 = 4/\pi^2$, i.e., $F(\omega)$ for $\phi = \pm\pi$ predominantly contains *two identical peaks symmetrically shifted in opposite directions* by π/τ. This case is known as "parity kicks."

For $\omega_a \simeq 0.95\omega_D$ (Fig. 1), the IPM scheme with $|\phi| \ll \pi$ is optimal, since the $k = 0$ peak then predominantly yields a spectral shift in the required positive direction towards the cutoff of $G_T(\omega)$, thereby suppressing R_e and R_g at longer τ than $\phi \simeq \pi$. The $|\phi| \ll \pi$ modulation can be used to suppress radiationless transitions in an impurity qubit embedded in a low-T solid [10]: if $\omega_a \simeq 0.95\omega_D \gtrsim 1$ GHz, dynamical Stark shifts

$\Delta \sim 0.1/\tau$, with $\tau \lesssim 100$ ps can take us beyond the cutoff of $G_T(\omega)$. *The RWA is seen to be inadequate,* at least for some modulations.

We turn now to proper dephasing when it dominates over decay. *The random frequency fluctuations* $\delta_r(t)$ in (5b) are typically characterized by a (single) correlation time t_r, with ensemble mean $\bar{\delta}_r = 0$. When the field $V(t)$ is used only for gate operations, we assume that it does not affect proper dephasing. The ensemble average over $\delta_r(t)$ results in Eqs. (5) with $\delta_r(t) = 0$ and no decay modulation [i.e., $\delta_a(t) = 0$ in Eq. (5b) and $K_{e(g)}(t, t') = 1$ in (6)], whereas $R(t) \rightarrow R(t) + R_d(t)$ with the dephasing rate

$$R_d(t) = \int_0^t dt' \Phi_r(t'), \qquad \Phi_r(t) = \overline{\delta_r(t)\delta_r(0)}. \qquad (10)$$

The dephasing CF $\Phi_r(t)$ is the counterpart of the bath CF $\Phi_T(t)$.

Assuming, for simplicity, that the decay is neglected and the control field $V(t)$ is resonant ($\omega_c = \omega_a$) with real envelope $V_0(t)$, we derive the ME for the qubit density matrix averaged over the random fluctuations $\delta_r(t)$. To this end, we transform the system to the rotating frame, write the pseudospin vector in spherical coordinates, $Q \equiv (Q_{-1}, Q_0, Q_1) = [\rho_{ge}, (\rho_{gg} - \rho_{ee})/\sqrt{2}, -\rho_{eg}]$, and tilt the frame to diagonalize the Hamiltonian of the TLS-field coupling [the last term in $H_S(t)$, Eq. (1)] by the transformation $Q_m = \sum_{m'} Q'_{m'} d^{(1)}_{m'm}(-\frac{\pi}{2})$, where $d^{(1)}_{m'm}(-\frac{\pi}{2})$ is the finite-rotation matrix for spin 1 [11]. In the tilted frame, the master equation at $t \gg t_r$ is

$$\begin{aligned} \dot{Q}'_{\pm 1} &= \{\pm i[V_0(t) + \Delta_d] - R_d/2\} Q'_{\pm 1}, \\ \dot{Q}'_0 &= -R_d Q'_0, \end{aligned} \qquad (11)$$

where we have made the secular approximation, which holds if $V_0(t) \gg R_d, |\Delta_d|$, and introduced $R_d = \lim_{t\to\infty} R_d(t)$, $\Delta_d = \lim_{t\to\infty} \Delta_d(t)$, the asymptotic real and imaginary parts of

$$R_d(t) + 2i\Delta_d(t) = \int_0^t dt' \Phi_r(t - t') \exp\left[i \int_{t'}^t V_0(t'') dt'' \right]. \qquad (12)$$

Equation (12) reveals the *analogy of dynamically modified dephasing to dynamically modified decay* [Eqs. (6)], both inferred from our unified treatment. For the validity of Eq. (11) it is necessary that $R_d, |\Delta_d| \ll 1/t_r$.

The *proper-dephasing* rate associated with $\Phi_r(t) = Ae^{-t/t_r}$ is $R_d = At_r$. In the presence of a *constant* V_0 [cw $V(t)$], it is modified according to Eq. (12) into

$$R_d = At_r/(V_0^2 t_r^2 + 1). \qquad (13)$$

For a sufficiently strong field, the dephasing rate R_d can be *suppressed* by the factor $1/(V_0 t_r)^2 \ll 1$. This suppression reflects the ability of strong, near-resonant Rabi splitting to shift the system out of the randomly fluctuating bandwidth, or average its effects. Quantum gate operations may be performed by *slight modulations* of the control field, which can flip the qubit without affecting proper dephasing. By comparison, a "bang-bang" method consisting of τ-periodic π pulses [5] is an analog of the above "parity kicks." Using the analog of Eq. (8), it can be shown to suppress R_d approximately according to Eq. (13) with $V_0 = \pi/\tau$. This bang-bang method requires pulsed fields with Rabi frequencies $\gg 1/\tau$, i.e., much stronger fields than the cw field in our Eq. (13). Using $t_r \sim 10^{-7}$ s, cw Rabi frequencies exceeding 1 MHz perform a significant dephasing suppression.

To conclude, our unified analysis has resulted in both principal and practical general conclusions: (i) Ultrafast modulations give rise to *antiresonant* (non-RWA) effects, manifest by "upward" ($|g\rangle \rightarrow |e\rangle$) transitions, that may significantly affect the decay rates into low-temperature baths. Nevertheless, decay suppression is possible under such conditions. (ii) Equations (8), (9), and (12) allow us to design *optimal* modulating pulses, i.e., the *lowest* pulse rate $1/\tau$ or the smallest dynamical Stark shifts Δ that can effect the suppression of decoherence.

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