Optimal Dynamical Decoherence Control of a Qubit

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A theory of dynamical control by modulation for optimal decoherence reduction is developed. It is based on the non-Markovian Euler-Lagrange equation for the energy-constrained field that minimizes the average dephasing rate of a qubit for any given dephasing spectrum.

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Introduction.— Quantum information processing (QIP) harbors enormous unleashed potential in the form of efficient algorithms for classically intractable tasks and unconditionally secure cryptography [1]. Perhaps the largest hurdle on the way to a realization of this potential is the problem of decoherence, which results when a quantum system, such as a quantum computer, interacts with an uncontrollable environment or bath [2]. Decoherence reduces the information processing capabilities of quantum computers to the point where they can be efficiently simulated on a classical computer. In spite of dramatic progress in the form of a theory of fault tolerant quantum error correction (QEC) [3], finding methods for overcoming decoherence that are both efficient and practical remains an important challenge. An alternative to QEC that is substantially less resource-intensive is dynamical decoupling (DD) [4, 5, 6]. In DD one applies a succession of short and strong pulses to the system, designed to stroboscopically decouple it from the environment. This can significantly slow down decoherence, though not halt it completely, since unlike QEC, DD does not contain an entropy removal mechanism. Similar in spirit to DD (in the sense of being feedback-free), but more general, is the method we term here “dynamical control by modulation” (DCM), wherein one may apply to the system a sequence of arbitrarily-shaped pulses whose duration may vary anywhere from the stroboscopic limit to that of continuous dynamical modulation [7, 8, 9, 10, 11, 12]. In the DCM approach, the decoherence rate is governed by a universal expression, in the form of an overlap between the bath-response and modulation spectra, subject to finite spectral bandwidth and amplitude constraints.

Neither DD [4, 5, 6] nor DCM [7, 12] studies have so far gone beyond particular schemes for suppression of decoherence. What is lacking is a systematic theory for finding the optimal modulation for any given decoherence process. Here we apply variational principles to the DCM approach in order to address this problem. We derive an equation for the optimal, energy-constrained control by modulation (ODCM) that minimizes dephasing, for any given dephasing spectrum. We numerically solve this equation, and compare the optimal modulation to energy-constrained DD pulses. We show that ODCM always outperforms DD when subjected to the same energy constraint. We note that Ref. [12] developed an optimal DD pulse sequence for the diagonal spin-boson model of pure dephasing, but without an energy constraint, i.e., assuming zero-width pulses. This was improved upon by perturbatively accounting for pulse widths in Ref. [13].

Model.— We consider a driven two-level system (qubit) with ground and excited states |g⟩ and |e⟩ separated by energy ω (we set ħ = 1), and Hamiltonian

\[ H(t) = (\omega_a + \delta_e(t)) |e⟩⟨e| + (V(t)|g⟩⟨e| + h.c.) , \]  

where \( V(t) = \Omega(t)e^{-i\omega_a t} + c.c. \) is a time-dependent resonant classical driving field with amplitude \( \Omega(t) \), and \( \delta_e(\omega) \) describes random, Gaussian distributed, zero-mean energy fluctuations. Let \( |ψ(t)⟩ \) denote the solution of the time-dependent Schrödinger equation with the Hamiltonian \( H(t) \), and let the density matrix \( ρ(t) = |ψ(t)⟩⟨ψ(t)| \) denote the corresponding ensemble average over realizations of \( \delta_e(t) \). We are interested in the average fidelity \( ⟨F(t)⟩ \), where \( ⟨\cdot\cdot\cdot⟩ \) is the average over all possible initial pure states of the fidelity \( F(t) = |⟨ψ(0)|ρ(t)|ψ(0)⟩| \). It can be shown that [12]:

\[ ⟨F(t)⟩ = 1 - α R(t)t \]  

\[ R(t) = 2\text{Re}\left(\int_{t_0}^{t_1} dt_2 \Phi(t_1 - t_2)e^{i(t_1)e(t_2)}\right)_{t}^{t_1} \]  

\[ \Phi(t) = \delta_e(t)\delta_e(0) \]  

\[ \epsilon(t) = e^{-i\int_{0}^{T} dt \Omega(t)} \]

where \( 0 < α \lesssim 1 \) is a known constant, \( ⟨\cdot\rangle_{t_0}^{t_1} \equiv \frac{1}{t_1 - t_0} ∫_{t_0}^{t_1} \cdot dt \) is the time-average, \( R(t) \) is the average modified dephasing rate, \( \Phi(t) \) is the second ensemble-average moment of the random (stationary non-Markov) noise, and \( \epsilon(t) \) is the phase factor associated with the modulation.

We impose the energy bound constraint

\[ ∫_{0}^{T} dt |Ω(t)|^2 = E \]

where \( T \) is the total modulation time and \( E \) is the energy constraint. As a boundary condition we require that the field is turned on, i.e. \( Ω(0) = 0 \).
Although the analysis below is given in the time-domain, it is advantageous to analyze the problem in the frequency domain, in terms of the universal expressions [7, 12]:

$$R(t) = 2\pi \int_{-\infty}^{\infty} d\omega G(\omega) F_t(\omega)$$

(6)

$$G(\omega) = (2\pi)^{-1} \int_{-\infty}^{\infty} d\Phi(t) e^{i\omega t}$$

(7)

$$F_t(\omega) = |\epsilon_t(\omega)|^2/t \quad \epsilon_t(\omega) = \frac{1}{\sqrt{2\pi}} \int_0^t dt_1 \epsilon(t_1)e^{i\omega t_1}$$

(8)

where $G(\omega)$ is the dephasing spectrum, $\epsilon_t(\omega)$ is the finite-time Fourier transform of the modulation function, and $F_t(\omega)$ is the normalized spectral modulation intensity.

The model we have just described applies to a qubit undergoing dephasing due to coupling to a finite-temperature bath of harmonic oscillators with energies $h\omega_{\lambda}$. The qubit then has an average modified dephasing rate (Fig. 2). However, since the energy constraint in the frequency domain is non-trivial we shall derive the equation of optimal control theory, e.g., [14, 15]. We apply where $\lambda$

$$\dot{\Phi}(t) = 0, \quad \Phi(t) = \int_0^t d\tau \Omega(\tau).$$

We shall show that the optimal modulation reduces the spectral overlap of the dephasing and modulation spectra (Fig. 2). However, since the energy constraint in the frequency domain is non-trivial we shall derive the equations for optimal modulation using the time domain.

**Optimization.**— We wish to find the optimal modulation, i.e., time-dependent near-resonant field, that minimizes $R(t)$. Calculus of variation is a widely used technique of optimal control theory, e.g., [14, 15]. We apply it to derive the Euler-Lagrange (EL) equations for the energy-constrained optimal modulation. The accumulated phase due to the modulation is $\phi(t) = \int_0^t d\tau \Omega(\tau)$. Let us write $\Phi(t) = \bar{\Phi}(t)e^{i\Delta t}$, where $\bar{\Phi}(t)$ and $\Delta$ are the amplitude and spectral center of the correlation function, respectively. Using Eqs. (2) and (3), we can then derive the EL equation for the optimal modulation (see Appendix A and B):

$$\lambda \ddot{\Phi}(t) = -Z[t, \phi(t)]$$

(11)

$$Z[t, \phi(t)] = \left\{ \Phi((t-t_1) \sin[\phi(t) - \phi(t_1) + \Delta(t-t_1)] \right\}^{t_1}_{t}$$

where $\lambda$ is the Lagrange multiplier. The boundary conditions for the accumulated phase are $\phi(0) = \phi(0) = 0$, which results in a smooth solution and accounts for turning the control field on. Eliminating $\lambda$ we find that the optimal control field shape is the solution to the following equation (see Appendix B):

$$\hat{\phi}(t) = \frac{-\sqrt{E}Z[t, \phi(t)]}{\sqrt{\int_0^T dt_1 \int_0^{t_1} dt_2 Z[t_2, \phi(t_2)]}}.$$ 

(12)

Equation (12) is the central result of this work. It furnishes the optimal time-dependent field amplitude, that maximizes the average fidelity $F(t)$ at the final time $T$, via $\Omega(t) = \hat{\phi}(t)$. Although Eq. 12 is a complicated non-linear integro-differential equation, it is very useful indeed, as we show next.

**Linearized EL equation.**— Assuming that we have a good initial guess $\phi_0(t)$ for the modulation, we can look for the optimal deviation $\nu(t)$ by writing $\phi(t) = \phi_0(t) + \nu(t)$, where $\nu(t) \ll 1$. Expanding Eq. (11) in powers of $\nu(t)$ and retaining only the first order, the linearized EL equation becomes (see Appendix C):

$$\lambda \ddot{\phi}(t) + (Q(t, t_1; \phi_0(t)) (\nu(t) - \nu(t_1)))|^{t_1}_{t} = -C(t; \phi_0, \lambda)$$

$$Q(t, t_1; \phi_0(t)) = \hat{\Phi}(t - t_1) \times$$

$$C(t; \phi_0(t), \lambda) = \lambda \ddot{\phi}_0(t) + Z[t, \phi_0(t)].$$

(13)

This linearized EL equation is valid also in the case of short time optimal modulation, for which we simply set $\phi_0(t) = 0$, subject to $\nu(t) \ll 1$ for $0 \leq t \leq T \ll 1$.

**Numerical analysis.**— Armed with the equations for the optimal modulation, we turn to solving them numerically for specific decoherence scenarios, defined by their dephasing spectra $G(\omega)$. We obtain the numerical solution to the integro-differential Eq. 12 via an iterative process, where we guess a probable solution that satisfies the boundary conditions and the constraint, use it in the RHS of Eq. 12 to compute the integral, and solve the resulting differential equation. The solution is then used in the RHS of Eq. 12, and so on.

For the examples presented below, we checked that several initial guesses converged to the same optimal modulation. Most importantly, we found that the optimal modulation is robust against random control field imperfections. This is due to the fact that the decoherence rate is determined by the accumulated phase and not the instantaneous modulation, Eq. 13. Specifically, we found that a 10% zero-mean random pulse fluctuation results in less than a 1% increase in the optimal dephasing rate.

We compare the optimal dephasing rate to the one obtained by the popular periodic DD control (“bang bang”) procedure [4], but to make the comparison meaningful we impose the same energy constraint. Finite-duration periodic DD against pure dephasing is the “bang bang” application of $n \pi$-pulses and is given in our setting by

$$\Omega(t) = \begin{cases} \pi/\nu & j\tau \leq t < j\tau + \nu \quad j = 0 \ldots n-1 \\ 0 & \text{otherwise} \end{cases}$$

(14)
where $\nu < \tau$ is the width of each pulse and $\tau$ is the interval between pulses. The energy constraint $E$ and the total modulation duration $T = \nu \tau + \nu$ are related via $n = \nu E / \pi^2$. In the frequency domain, the spectral modulation intensity can be described by a series of peaks, where the two main peaks are at $\pm \pi / \tau$. Thus, the peaks are shifted in proportion to the energy invested in the modulation. However, DD is not an admissible solution to our EL equation due to its discontinuous derivative. In order to improve the comparison, we apply our linearized EL equation with the DD modulation as an initial guess, and obtain the optimal modulation in the vicinity of the DD control.

(a) Single-peak resonant dephasing spectrum.— This simple dephasing spectrum describes a common scenario where $\Phi(t) = e^{-t/t_{e}}$, where $\gamma$ is the long-time dephasing rate $[R(t \to \infty) = 2\pi \gamma]$ and $t_{e}$ is the noise correlation time. Fig. 1(a) shows $R(T)$, normalized to the bare (unmodulated) dephasing rate, as a function of the energy constraint. As expected, the more energy is available for modulation, the lower is the dephasing rate. For low energies the optimal modulation significantly outperforms DD, while at higher energies this difference disappears. These results can be understood from Fig. 2(a), by noticing that the two central DD peaks have significant overlap with $G(\omega)$ at the low energy value shown. As $E$ is increased at fixed $T$ the DD peaks move farther apart, and have less overlap with $G(\omega)$, leading to improved performance. Applying the linearized EL equation with DD as initial guess yields only mild improvements (not shown). The explanation for the superior performance of the optimal modulation is also evident from Fig. 2(a): since higher frequencies have lower coupling strength in this case, the optimal control “reshapes” so as to maximize its weight in the high-frequency range, to the extent permitted by the energy constraint. The modulation can be well approximated by $\Omega(t) = a[1 + e^{-t/T}(t/T - 1)]$, where $a$ is determined by the energy constraint, which fits the inset in Fig. 1(a).

(b) Single-peak off-resonant dephasing spectrum.— This dephasing spectrum describes a variation on the aforementioned scenario, where the spectral peak is shifted $[\Delta \neq 0 \in \Phi(t) = \Phi(t)e^{i\Delta\tau}]$, e.g., coupling to a non-resonant bath. With no other constraints, the optimal modulation is trivially similar to the one of the resonant spectrum, with a shifted energy-constraint $E_{\text{opt}}^{\text{off-res}} = E_{\text{res}}^{\text{opt}} + \Delta$. However, by imposing a positivity constraint, $\Phi(t) \geq 0$ (positive field amplitude), one obtains non-trivial behavior of $R(T)$ as a function of the energy constraint – see Fig. 1(b). Here we used the linearized EL equation with the DD modulation [14] as an initial guess. For both the DD and optimal modulations, we observe an initial increase in the dephasing rate as a function of energy, followed by a decrease. For DD, this can be interpreted as a manifestation of the initial anti-Zeno effect and the subsequent quantum Zeno effect [7, 10]. Because of the positivity constraint, the optimal modulation does worse than the unmodulated case, for low enough energy. The DD modulation is optimal for small energy constraints, hence the decoherence rates of DD and our optimal solution coincide. This is because the DD peaks do not overlap the off-resonant spectral peak. However, as the positive-frequency main DD peak [Fig. 2(b)] nears the off-resonant spectral peak, with increased energy, the optimal modulation diverges from the DD modulation, and “reshapes” itself so as to couple to higher modes of the bath. In the time domain [Fig. 1(b) inset], this is seen as a smoothing of the abrupt DD modulation. At even higher energy constraints, there is once more no improvement by the optimal modulation over DD, yet there is an improvement over the unmodulated case. Over the entire range of $E$, the optimal modula-
tion results in a much flatter $R(T)$ than DD, which is an indicator of its robustness. While DD is strongly influenced by the off-resonant peak, the optimal modulation exploits the energy available to find the minimal overlap, irrespective of dephasing spectrum.

(c) 1/f dephasing spectrum.— The ubiquitous 1/f dephasing spectrum that describes a variety of experiments—e.g., charge noise in superconducting qubits [16]—is given in our notation by $G(\omega) \propto 1/\omega$, with cutoffs $\omega_{\text{min}}$ and $\omega_{\text{max}}$. Fig. I(c) shows that as expected, the more energy is available for modulation, the lower the dephasing rate. Since, as in case (a), higher frequencies now have lower coupling strength, the optimal control “reshapes” so as to have as high a weight in the high frequency range as the energy constraint allows [Fig. 2(c)]. This is expressed in the time-domain [Fig. I(c) inset] as the initial increase in the modulation strength ($t < 50$). The later decrease in modulation strength can be attributed to the lower cutoff, where the optimal modulation benefits from lower frequencies, i.e., lower modulation amplitudes. Upon comparing the 1/f case to the Lorentzian spectrum, Fig. I(a), we observe a similar optimal initial chirped modulation in the time domain. Despite the differences in the long-time behavior (due to the lower cutoff in the 1/f case), these two examples allow us to generalize to any dephasing spectrum with a monotonically decreasing system-bath coupling strength as a function of frequency. The optimal modulation for such spectra will be an energy-constrained chirped modulation, with variations due to other spectral characteristics, e.g., cutoffs.

(d) Multi-peaked dephasing spectrum.— This describes the most general scenario, where there can be several resonances and noise correlation times. Fig. I(d) shows $R(T)$ as a function of the energy constraint. Once again, because DD does not account for the dephasing spectrum, its performance is much worse than the optimal modulation, whose “reshaping” results in monotonically improving performance: the peaks of the optimal modulation are predominantly anti-correlated with the peaks of $G(\omega)$.

Conclusions.— We have found the optimal modulation for countering pure dephasing upon imposing an energy constraint on the DCM approach [7, 12], by deriving and solving the Euler-Lagrange equation (12). This yields optimal reduction of the overlap of the dephasing and the modulation intensity spectra. We stress that our optimal control theory results are also applicable to scenarios other than pure dephasing, such as amplitude noise (relaxation), due to the universality of Eqs. (2)-(8). The form of the energy constraint will then differ in detail from the pure dephasing case. However, our general conclusions about the optimal modulation to minimize spectral overlap, will remain valid. We expect that the optimal modulation technique will find useful applications in quantum information processing and quantum computation. The price is that one must acquire intimate knowledge of the noise spectrum, which is often neglected, as previous control techniques such as DD and QEC had no use for it. We have shown that this information can result in the maximization of fidelity, under operational constraints.

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APPENDIX A: GENERAL COMMENTS ON DERIVING OPTIMAL FUNCTIONS

For the optimal control of a functional

\[ F(y, \dot{y}) = \int_0^T dt F(t, y, \dot{y}) \]  

(A1)

with the constraint

\[ K(y, \dot{y}) = \int_0^T dt K(t, y, \dot{y}) = E \]  

(A2)

one follows the following procedure:

(i) Solve the Euler-Lagrange equation:

\[ \frac{\delta F}{\delta y} - \frac{\partial}{\partial t} \frac{\delta F}{\delta \dot{y}} = -\lambda \left[ \frac{\delta K}{\delta y} - \frac{\partial}{\partial t} \frac{\delta K}{\delta \dot{y}} \right] \]  

(A3)

where \( \delta F \) is the variation of \( F \), \( \lambda \) is the Lagrange multiplier, and the boundary conditions are \( y(0) = y_0 \) and \( \dot{y}(0) = \dot{y}_1 \).

(ii) Insert the solution \( \tilde{y}(t; \lambda) \) into the constraint:

\[ K(\tilde{y}(t; \lambda), \tilde{\dot{y}}(t; \lambda)) = E \]  

(A4)

and obtain \( \lambda = \lambda(E) \).

(iii) Eliminate \( \lambda \) by inserting \( \lambda(E) \) into \( \tilde{y}(t; \lambda) \) and obtain the optimal solution, \( \tilde{y}(t; E) \), that minimizes the functional \( F \), under the constraint \( K = E \).

APPENDIX B: DERIVATION OF THE EULER-LAGRANGE EQUATION

The average modified decoherence rate is given by:

\[ R(T) = \frac{2}{T} \int_0^T dt \int_0^t dt_1 \Phi(t - t_1) \cos[\phi(t) - \phi(t_1) + \Delta(t - t_1)] \]  

(B1)

\[ = \frac{2}{T} \int_0^T dt \int_0^T dt_1 \Theta(t - t_1) \Phi(t - t_1) \cos[\phi(t) - \phi(t_1) + \Delta(t - t_1)] \]  

(B2)

where \( \Theta(t) \) is the Heaviside step function.

One arrives at the following variation of the average modified decoherence rate:

\[ \delta R(T) = \frac{2}{T} \int_0^T dt \int_0^T dt_1 \]  

\[ \left[ -\Theta(t - t_1) \Phi(t - t_1) \sin[\phi(t) - \phi(t_1) + \Delta(t - t_1)] \delta \phi(t) \right. \]

\[ + \Theta(t - t_1) \Phi(t - t_1) \sin[\phi(t) - \phi(t_1) + \Delta(t - t_1)] \delta \phi(t_1) \]

(B3)

\[ = \frac{2}{T} \int_0^T dt \int_0^T dt_1 \]  

\[ \left[ -\Theta(t - t_1) \Phi(t - t_1) \sin[\phi(t) - \phi(t_1) + \Delta(t - t_1)] \delta \phi(t) \right. \]

\[ - \Theta(t_1 - t) \Phi(t_1 - t) \sin[\phi(t) - \phi(t_1) + \Delta(t - t_1)] \delta \phi(t) \]

(B4)

\[ = \frac{2}{T} \int_0^T dt \int_0^T dt_1 \left[ -\Phi(|t - t_1|) \sin[\phi(t) - \phi(t_1) + \Delta(t - t_1)] \delta \phi(t) \right. \]

\[ \left. + \Phi(|t - t_1|) \sin[\phi(t) - \phi(t_1) + \Delta(t - t_1)] \delta \phi(t_1) \right] \]  

(B5)

where we have made a \( t \leftrightarrow t_1 \) substitution in the second integrand of Eq. (B3), and notice that \( \Theta(t)f(t) + \Theta(-t)f(-t) = f(|t|) \).
One can easily see that defining the constraint functional as:

$$K(t, \phi(t), \dot{\phi}(t)) = \int_0^t dt_1 |\dot{\phi}(t_1)|^2 = E,$$  \hspace{1cm} (B6)

with $K(t, \phi(t), \dot{\phi}(t)) = |\dot{\phi}(t_1)|^2$ results in the variation:

$$\delta K = 2\dot{\phi}(t)\delta\dot{\phi}(t).$$  \hspace{1cm} (B7)

Combining Eqs. (B5), (B7) and (A3) results in the Euler-Lagrange equation:

$$\lambda \ddot{\phi}(t) + Z[t, \phi(t)] = 0$$  \hspace{1cm} (B8)

where

$$Z[t, \phi(t)] = \frac{1}{T} \int_0^T dt_1 \tilde{\Phi}(|t - t_1|) \sin[\phi(t) - \phi(t_1) + \Delta(t - t_1)].$$  \hspace{1cm} (B9)

**APPENDIX C: DERIVATION OF THE LINEARIZED EULER-LAGRANGE EQUATIONS**

In some cases it is advantageous to linearize the EL equations with respect to the modulation. If one looks for the optimal deviation $\nu(t)$ from a given pulse shape, $\phi_0(t)$, then one can write $\phi(t) = \phi_0(t) + \nu(t)$, where $\nu(t) \ll 1$. Equation (B8) then becomes:

$$\lambda(\ddot{\phi}_0(t) + \ddot{\nu}(t)) = -\frac{1}{T} \int_0^T dt_1 \tilde{\Phi}(|t - t_1|) \left[ \sin[\phi_0(t) - \phi_0(t_1) + \Delta(t - t_1)] \cos[\nu(t) - \nu(t_1)] ight. \\
\left. + \cos[\phi_0(t) - \phi_0(t_1) + \Delta(t - t_1)] \sin[\nu(t) - \nu(t_1)] \right]$$

$$= -\frac{1}{T} \int_0^T dt_1 \tilde{\Phi}(|t - t_1|) \left[ \sin[\phi_0(t) - \phi_0(t_1) + \Delta(t - t_1)] \right. \\
\left. + \cos[\phi_0(t) - \phi_0(t_1) + \Delta(t - t_1)] \sin[\nu(t) - \nu(t_1)] \right] + O(\nu^2(t))$$  \hspace{1cm} (C1)

where we approximated $\sin[\nu(t) - \nu(t_1)] \approx \nu(t) - \nu(t_1) + O(\nu^3(t))$ and $\cos[\nu(t) - \nu(t_1)] \approx 1 - \frac{1}{2}(\nu(t) - \nu(t_1))^2 + O(\nu^4(t))$. The linearized Euler-Lagrange equation becomes:

$$\lambda \ddot{\nu}(t) + \frac{1}{T} \int_0^T dt_1 Q(t, t_1; \phi_0(t)) (\nu(t) - \nu(t_1)) = -C(t; \phi_0, \lambda)$$  \hspace{1cm} (C3)

where

$$Q(t, t_1; \phi_0(t)) = \tilde{\Phi}(|t - t_1|) \cos(\phi_0(t) - \phi_0(t_1) + \Delta(t - t_1))$$  \hspace{1cm} (C4)

$$C(t; \phi_0(t), \lambda) = \lambda \ddot{\phi}_0(t) + Z[t, \phi_0(t)].$$  \hspace{1cm} (C5)