Empirical determination of dynamical decoupling operations

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Strong and fast ''bang-bang'' (BB) pulses have been recently proposed as a means for reducing decoherence in a quantum system. So far theoretical analysis of the BB technique relied on model Hamiltonians. Here we introduce a method for empirically determining the set of required BB pulses, that relies on quantum process tomography. In this manner an experimenter may tailor his or her BB pulses to the quantum system at hand, without having to assume a model Hamiltonian. In addition, the previous work has been extended to a general noiseless evolution via the stabilizer formalism.

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I. INTRODUCTION

Quantum computers hold great promise in solving certain computational problems faster than their classical counterparts, but they are notoriously susceptible to decoherence (deviations from unitary dynamics) and unitary errors, the combination of which we refer to as ''noise.'' The effect of decoherence is to induce computational errors that destroy the quantum speed-up: a decohered quantum computer can be efficiently simulated by a classical computer [1]. Hence the ultimate success of quantum information processing depends on the ability to implement error correction or avoidance techniques. To this end, a variety of quantum error correcting codes (QECC) and other methods have been designed. These methods all share an important feature: they are designed to deal with *specific models* of errors, as embodied in an assumed system-bath interaction Hamiltonian. The class of active (e.g., stabilizer) QECC [2–5], for example, is designed to correct independent errors resulting from (up to) some fixed number, t, of system-bath many-body interactions; the class of passive QECC (decoherence-free subspaces) works optimally under the assumption of collective (i.e., fully correlated) decoherence [6–10] or assumes multiple-qubit errors [11]; dynamical decoupling or symmetrization methods assume baths with relatively long correlation times and weak system-bath coupling, so that decoherence may be suppressed using fast and strong ''bang-bang'' (BB), or dynamical decoupling, pulses, introduced in Ref. [12], and further developed in Refs. [13–29]. One may also note that BB pulses are related to the so-called average Hamiltonian theory [54], and are important for the ability to simulate one system by another [25,29–31]. In spite of this impressive arsenal of methods there is a fundamental problem in the model-specific approach in terms of its applications to experimental quantum information processing. The problem is that in real world applications, decoherence is often a combined effect, which arises from a variety of sources, and does not correspond to one particular model. It is often very difficult to identify and isolate the various sources. The result is that the model-dependent approach for overcoming decoherence breaks down when applied to realistic systems, since it inevitably fails to capture all sources. In addition, current methods tend to ignore the experimental constraints imposed by the finiteness of resources, such as the scarcity of qubits in present-day implementations of quantum computers (presently, fewer than 10 qubits). Of course, this criticism in no way diminishes the importance of the model-specific approach: it is through that approach that ground-breaking new results have been obtained which establish the in-principle possibility of overcoming decoherence. In particular, this work has led to the observation that fault tolerant quantum computation is possible in the independent errors model, provided the fidelity of gate operations is above a certain threshold [32–36].

We focus here on the BB method and consider a paradigm that is the reverse of the model-dependent approach to decoherence reduction: Instead of assuming a specific model of decoherence, designing a corresponding QECC, and then looking for a system that might be described to a good approximation by that model, *we propose to tailor a set of* BB *pulses to a system, from experimentally measured decoherence data*. We call this approach, which we introduced first in Ref. [26], ''empirical bang-bang.'' Empirical BB is a phenomenological approach which forsakes a microscopic understanding of the underlying decoherence processes in favor of a direct attack on the combined effect of all sources of decoherence at once. This method aims to achieve an optimized control [37–40] by using a closed-loop learning algorithm [41–43]. This closed-loop method, first introduced in Ref. [41], and only recently discussed as a method of decoherence management [43], can be used to iteratively optimize the output taking into account practical constraints imposed by the specific physical and experimental realization.

That empirical BB is feasible, in principle, follows from two key facts: (i) It is possible to experimentally measure the superoperator (i.e., the map that propagates the density matrix) characterizing the noise in a particular system by using quantum process tomography (QPT); (ii) As we show here, given knowledge of the superoperator it is possible to design a BB procedure. Thus an experiment can, in principle, provide all the information needed to design an optimized set of BB pulses.

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This paper is arranged as follows. In Sec. II we review the basic background to quantum process tomography, and the theory for decoupling by symmetrization. We then present, in Sec. III, a derivation and discussion of several formulas for determining the set of decoupling operations. In Sec. IV we generalize the entire scheme to operations on *encoded* qubits in terms of the geometric picture which is a quite general and new result. It establishes a method for designing a QECC and/or a decoherence-free subspace (DFS) for a given set of BB pulses, or choosing the necessary set based on an encoding. These basic methods are illustrated in Sec. V with a few examples. We then indicate in Sec. VI how the empirically determined set of BB pulses can be optimized using a learning-loop algorithm.

II. REVIEW

In this section we review the important components of the empirical determination of bang-bang operations. These include QPT, the theory of dynamical decoupling operations for a given Hamiltonian, and its geometrical interpretation. Readers familiar with these concepts can choose to skip ahead to Sec. III, although the notation introduced in this section will be used in the remainder of the paper.

A. Quantum process tomography

The dynamics of an open quantum system coupled to a bath is formally obtained from the time-ordered evolution

$$U(t)=\mathcal{T}\exp\left[-i\int^{t}H(t')dt'\right], \tag{1}$$

under the combined system-bath Hamiltonian

$$H=H_S\otimes I_B+I_S\otimes H_B+H_{SB},$$

$$H_{SB}=\sum_{\gamma}S_\gamma\otimes B_\gamma, \tag{2}$$

where I is the identity operator, H_S is the Hamiltonian for the system alone, H_B is the Hamiltonian for the bath alone, H_{SB} is the system-bath interaction Hamiltonian, and the S_γ and B_γ are operators on the system and the bath, respectively. Tracing over the bath degrees of freedom in order to obtain the time-evolved system density matrix

$$\rho(t)=\mathrm{Tr}_B[U(t)(\rho(0)\otimes\rho_B(0))U^{\dagger}(t)], \tag{3}$$

where $\rho(0)$ is the initial density matrix of the (open) system, $\rho_B(0)$ is the initial density matrix of the bath. It can be shown that this agrees with the most general quantum evolution consistent with the condition of complete positivity, known as the Kraus operator sum representation (OSR) [44–46]:

$$\begin{aligned}\mathcal{E}_t(\rho(0))\equiv\rho(t)&=\sum_{\mu\nu}A_{\mu\nu}(t)\rho(0)A_{\mu\nu}^{\dagger}(t)\\&=\sum_{\alpha,\beta}\chi_{\alpha,\beta}(t)K_\alpha\rho(0)K_\beta^{\dagger}.\end{aligned} \tag{4}$$

The *Kraus operators* can be related to Eq. (3) through

$$A_{\mu\nu}(t)=\sqrt{\lambda_\nu}\langle\mu|U(t)|\nu\rangle, \tag{5}$$

where $|\nu\rangle,|\mu\rangle$ are eigenvectors of the initial bath density matrix: $\rho_B(0)=\Sigma_\nu\lambda_\nu|\nu\rangle\langle\nu|$ [47]. Since $\mathrm{Tr}[\rho(t)]=1$, they satisfy the normalization condition: $\Sigma_\mu A_{\mu\nu}^{\dagger}A_{\mu\nu}=I_S$. The matrix

$$\chi_{\alpha,\beta}(t)=\sum_{\mu\nu}b_{\mu\nu;\alpha}b_{\mu\nu;\beta}^{*}$$

is a time dependent, Hermitian coefficient matrix defined by a transformation of the Kraus operators to a *fixed* (i.e., time-independent) operator basis K_α,

$$A_{\mu\nu}(t)=\sum_{\alpha}b_{\mu\nu;\alpha}(t)K_\alpha.$$

A prescription for determining the superoperator $\mathcal{E}_t$ from experimental data (QPT) was given in a number of recent papers [48–50], and has very recently been applied in NMR experiments [51]. *In this paper we will take QPT to mean the determination of the coefficient matrix $\chi_{\alpha\beta}(t)$, with respect to a given (experimentally convenient) choice of fixed basis operators K_α.* Formally, the problem is to invert the χ matrix from experimental data. Since χ is time dependent, it is clear that one can in practice only sample it. If the decoherence process is Markovian then it suffices to obtain the time-independent coefficient matrix $a_{\alpha\beta}$ that appears in the Lindblad equation [47,52,53]. However, even this is a formidable problem: if the density matrix has dimensions $N\times N$ (where for n qubits $N=2^n$) then a simple counting argument shows that there are at most N^4-N^2 independent real parameters in $a_{\alpha\beta}$ and the same number, but time dependent in χ. Even for one qubit this amounts to 12 different parameters that may have to be measured to completely characterize the decoherence process. Fortunately, it is well known that in practice as few as 2 parameters may suffice, as is the case with the T_1 and T_2 relaxation times in NMR [54].

The general idea behind QPT is to characterize the superoperator action on a complete basis set. To see this, let the N^2 matrices ρ_j be a basis for the density matrix ρ. For example, ρ_j could be the set of pure states $|j\rangle\langle j'|$, which are then fed into the decoherence process as inputs: $\mathcal{E}(\rho_j)=\Sigma_k\lambda_{jk}\rho_j$. Using quantum state tomography [55], one can experimentally determine λ_{jk}, which fully specifies the superoperator $\mathcal{E}$, since it is now possible to find the χ matrix: Define ξ by $K_\alpha\rho_jK_\beta^{\dagger}=\Sigma_k\xi_{jk}^{\alpha\beta}\rho_k$, where K_α are the fixed basis Kraus operators. Then one can show that $\Sigma_{\alpha\beta}\xi_{jk}^{\alpha\beta}\chi_{\alpha\beta}=\lambda_{jk}$ [49]. This can be thought of as a matrix equation for

the vector χ and it can be solved by computing the inverse of the matrix ξ. Thus, by measuring λ and by giving ξ through a choice of the fixed operator basis K_α, finding the χ matrix has been transformed into a linear algebra problem. In practice, we note that it may often be difficult to prepare the full basis set ρ_j. An interesting alternative, using entangled input states, was recently proposed in Ref. [56]. A method that circumvents tomography altogether (but is less general), using quantum network ideas, was described in Ref. [57].

B. Decoupling by symmetrization

The process of decoupling by symmetrization counteracts noise by applying sequences of frequent and strong pulses. The time scales are crucial: one needs to perform a complete cycle of symmetrization operations in a time shorter than τ_c, the inverse of the high-frequency cutoff of the bath spectral density [12–14]. An elegant group-theoretical treatment shows that the applied pulses are unitary transformations forming a finite-dimensional group, and the application of a series of pulses amounts to an average (symmetrization) over this group [15–19]. A geometrical interpretation, reviewed below, can offer further insight [24]. The method can also be used to perform " environment engineering," in order to prepare the conditions that allow for DFSs [15,19,27], as well as in order to eliminate leakage errors that couple encoded states with states out of a DFS [15,28]. We briefly review this theory.

A set of symmetrization operations is chosen such that they form a discrete subgroup of the full unitary group of operations on the Hilbert space of the system. Denote this group $\mathcal{G}$ and its elements g_j, $j=0,1,\ldots,|\mathcal{G}|-1$, where $|\mathcal{G}|$ is the order of the group. The cycle time is $T_c=|\mathcal{G}|\Delta t$, where $|\mathcal{G}|$ is the number of symmetrization operations, and Δt is the time that the system evolves freely between operations under $U_0=\exp(-iHt)$ with H given by Eqs. (2). The symmetrized evolution is given by

$$U(T_c)=\prod_{j=0}^{|\mathcal{G}|-1} g_j^\dagger U_0(\Delta t) g_j \equiv e^{iH_{\rm eff}T_c},$$

where the evolution under $H_{SB}+H_B$ has been neglected during pulse application, i.e., during the action of the group elements g_j. $H_{\rm eff}$ denotes the resulting effective Hamiltonian. Since the approximation requires very strong, short pulses to be implemented in a sequence, they have been termed as BB operations (we will use decoupling, symmetrization, and BB operations interchangeably). In this (BB) limit

$$H \mapsto H_{\rm eff}=\frac{1}{|\mathcal{G}|}\sum_{j=0}^{|\mathcal{G}|-1} g_j^\dagger H g_j \equiv \Pi_{\mathcal{G}}(H), \tag{6}$$

where $H_{\rm eff}$ is the desired Hamiltonian (without noise). The map $\Pi_{\mathcal{G}}$ is the projector into the centralizer $Z(\mathcal{G})$ defined as

$$Z(\mathcal{G})=\{X|[X,g_j]=0, \quad \forall \ g_j\in\mathcal{G}\}.$$

The resulting effective Hamiltonian now satisfies $[H_{\rm eff},\mathcal{G}=0]$, so that if $\mathcal{G}$ is generated by $\{I,H_S,S_\gamma\}$, the evolution will proceed without the operators S_γ affecting the system, since the error operators will commute with the effective Hamiltonian. The *control algebra* is the algebra generated by the set $\{g_j\}$. Even if the symmetrization is performed under less than ideal conditions, BB can still reduce the noise in the system [12,13].

The main advantage offered by dynamical decoupling is that *it does not require extra qubits*. This is a very attractive feature compared to both active and passive error correction, one that may make dynamical decoupling a method of choice for small-scale quantum computer implementations, provided its stringent time-scale requirements can be met.

C. Geometry of the decoupling method

In preparation for the remainder of the paper, and as an intuitive aid, we briefly review the geometric description of BB controls developed in Ref. [24]. Let us explicitly introduce $N\equiv n^2-1$ traceless, Hermitian generators $\{\lambda_i\}_{i=1}^N$ of SU(n). These generators are closed under commutation and span the space of traceless Hermitian matrices. For SU(2), the Pauli matrices are commonly used; for SU(3), the Gell-Mann matrices, and for higher dimensions, one may use a direct generalization of the Gell-Mann matrices. For dimensions that are a power of two (and quantum computing) it is often convenient to use the Pauli group (tensor products of Pauli matrices). The $\{\lambda_i\}$ satisfy trace orthogonality

$$\mathrm{Tr}(\lambda_i\lambda_j)=M\delta_{ij}, \tag{7}$$

where M is a normalization constant (often taken to be 2 for Lie algebras or n for $n\times n$ matrices). Expanding the system operators in terms of the $\{\lambda_i\}$ yields

$$K_\gamma=\sum_i a_{i\gamma}\lambda_i, \tag{8}$$

where the expansion coefficients are

$$a_{i\gamma}=\frac{1}{M}\mathrm{Tr}(\lambda_i K_\gamma). \tag{9}$$

Using this, H_{SB} can be written as follows:

$$\begin{aligned} H_{SB}&=\sum_\gamma S_\gamma\otimes B_\gamma \\ &=\sum_\gamma\sum_{i=1}^{N} a_{i\gamma}\lambda_i\otimes B_\gamma \\ &\equiv\sum_\gamma (\vec{a}_\gamma\cdot\vec{\lambda})\otimes B_\gamma. \end{aligned} \tag{10}$$

Here $\vec{a}_\gamma$ and $\vec{\lambda}$ are vectors of length N. In this coherence vector representation, used extensively in Ref. [58], an $n\times n$ Hamiltonian H is a vector with coordinates $\vec{a}_\gamma$ for each error γ in an N-dimensional vector space spanned by the $\{\lambda_i\}$ as basis vectors, with ordinary vector addition and scalar multiplication. The open system evolution is thus described by a vector (or vector field) in the space of possible evolutions.

Now, as is well known, there is a homomorphic mapping between the Lie groups SU(2) and SO(3) [59]. This mapping is generalized as follows for SU(n) and a subgroup of the rotation group SO(N):

$$U_k^\dagger \lambda_i U_k = \sum_{j=1}^{N} R_{ij}^{(k)} \lambda_j , \tag{11}$$

where the matrix $R^{(k)} \in \mathrm{SO}(N)$, the adjoint representation of SU(n).

The BB operation [Eq. (6)] may now be viewed as a weighted sum of rotations of the (adjoint) vectors $\vec{a}_\gamma$. To see this, first let

$$\vec{a}_\gamma^{(k)} = R^{(k)} \vec{a}_\gamma . \tag{12}$$

This represents the rotation by $R^{(k)}$ of the coordinate vector $\vec{a}_\gamma$. Next average over all rotations

$$\vec{a}'_\gamma = \frac{1}{|\mathcal{G}|} \sum_{k=0}^{|\mathcal{G}|-1} \vec{a}_\gamma^{(k)} . \tag{13}$$

Finally, note that the effective Hamiltonian, after the BB operations, can be rewritten as

$$H_{\mathrm{eff}} = \frac{1}{|\mathcal{G}|} \sum_{k=0}^{|\mathcal{G}|-1} U_k^\dagger H U_k = \sum_\gamma (\vec{a}'_\gamma \cdot \vec{\lambda}) \otimes B_\gamma . \tag{14}$$

Equation (14) [compared to Eq. (10)] is the desired geometric representation of BB operations. Their effect is to simply transform, for each error γ, the coordinates $\vec{a}_\gamma$ to $\vec{a}'_\gamma$. It is simplest to interpret this in the case of storage, where we seek BB operations such that $H_{\mathrm{eff}} = 0$. Since the errors can be decomposed in the linearly independent basis set indexed by γ, each term $\vec{a}'_\gamma \cdot \vec{\lambda}$ must vanish separately. Furthermore, since the λ_i are independent this can only be satisfied if $\vec{a}'_\gamma = \vec{0}$ for each γ. This means that

$$\vec{a}'_\gamma = \left(\frac{1}{|\mathcal{G}|} \sum_k R^{(k)} \right) \vec{a}_\gamma = \vec{0}, \tag{15}$$

i.e., the sum of all rotations applied to the original coordinate vector $\vec{a}_\gamma$ must vanish.

Similarly, to obtain a modified evolution corresponding to a target Hamiltonian $H_{\mathrm{eff}}^t = \Sigma_\gamma (\vec{a}_\gamma^t \cdot \vec{\lambda}) \otimes B_\gamma$, we require the weighted sum of rotations applied to the original coordinate vector to be equal to the corresponding target coordinate vector $\vec{a}_\gamma^t$. That is, for $H_{\mathrm{eff}} \neq 0$, the following condition should be satisfied to obtain the desired evolution:

$$\vec{a}'_\gamma = \vec{a}_\gamma^t . \tag{16}$$

This may require a combination of switching strategies for the BB pulses [19].

It should be noted that the geometrical picture is an explicit representation of a subset of the group algebra $\mathbb{C}\mathcal{G}$ using the set of traceless Hermitian matrices and the identity as the basis. When the coefficients of the adjoint vector are real, the resulting matrix H_{eff} is Hermitian. When they are complex, the resulting matrix is not Hermitian and the evolution is not unitary, but may still be treated empirically, as we show below.

We now turn to show how to find the BB pulses directly from experimental data, i.e., given a QPT measurement of the χ matrix.

III. DETERMINATION OF DECOUPLING OPERATORS

Since the BB method operates at extremely fast time scales it is useful to consider a short-time expansion of the OSR evolution equation (4). To do so we follow [47,60], where it was shown how the OSR can be rewritten to resemble the Lindblad equation [52,53]. Thus, the OSR can be rewritten as

$$\rho(t) = \rho(0) - \frac{i}{\hbar}[S(t), \rho(0)] + \frac{1}{2} \sum_{\alpha,\beta=1}^{N} \chi_{\alpha,\beta}(t) \times \{ [K_\alpha, \rho(0) K_\beta^\dagger] + [K_\alpha \rho(0), K_\beta^\dagger] \}, \tag{17}$$

where $S(t)$ is the Hermitian operator defined by

$$S(t) = \frac{i\hbar}{2} \sum_{\alpha=1}^{N} [\chi_{\alpha,0}(t) K_\alpha - \chi_{0,\alpha}(t) K_\alpha^\dagger]. \tag{18}$$

Note the similarity of Eq. (17) to the Lindblad equation [52,53]. Indeed, the Lindblad Markovian semigroup master equation can be derived from Eq. (17) via a coarse-graining procedure [47,60], which replaces the time-dependent $\chi_{\alpha,\beta}$ matrix elements with their time averages over an interval that is longer than the bath correlation-time τ_c, and thus longer than the BB time scale. An important outcome of this procedure is that the coarse-grained $S(t)$ can be interpreted as a system Hamiltonian H_S plus a Lamb shift correction [47,60]. While still exact, Eq. (17) is more amenable to a short-time expansion than the original (equivalent) form of the OSR, Eq. (4).

Note that the "fixed basis" $\{K_\alpha\}_{\alpha=1}^N$ is completely analogous to the Hermitian generators $\{\lambda_i\}_{i=1}^N$ of SU(n) used in the geometric picture of Sec. II C. Thus, assuming a Hermitian basis $\{K_\alpha\}$ we can rewrite Eq. (18) as

$$S(t) = i\hbar \sum_{\alpha=1}^{M} \mathrm{Im}[\chi_{\alpha,0}(t)] K_\alpha = i\hbar\, \mathrm{Im}(\vec{\chi}) \cdot \vec{K},$$

which can be interpreted as giving the "Hamiltonian" $S(t)$ as a vector with coordinates $\mathrm{Im}[\chi_{\alpha,0}(t)]$ in a space with basis vectors $\{K_\alpha\}$.

Next we give a general method for determining BB controls from empirical data, specialize the applicability of this method somewhat, and then treat storage, single-qubit operations, and computation.

A. Empirical bang-bang condition

Before going into a detailed and more careful analysis, we first present a ''rough'' version of the empirical BB condition. We note two key facts: (i) in a first-order decoupling scheme [16], the BB method will operate only to undo the undesired evolution due to $S(t)$; (ii) from Secs. II A and II B we find that, under the action of BB controls, the $\{K_\alpha\}$ transform as

$$\begin{aligned} K_\alpha &\overset{\mathrm{BB}}{\rightarrow} \frac{1}{|\mathcal{G}|}\sum_k U_k^\dagger K_\alpha U_k \\ &= \frac{1}{|\mathcal{G}|}\sum_k \sum_{\beta=1} R^{(k)}_{\alpha\beta} K_\beta \\ &= \frac{1}{|\mathcal{G}|}\sum_k (R^{(k)}\vec{K})_\alpha . \end{aligned} \tag{19}$$

Thus, given the considerations above concerning the effect of BB pulses and their geometrical interpretation, we can express the BB-modified open system evolution as

$$\begin{aligned} S &= i\hbar\,\mathrm{Im}(\vec{\chi})\cdot\vec{K} \\ &\overset{\mathrm{BB}}{\rightarrow} \mathrm{Im}(\vec{\chi})\cdot\frac{1}{|\mathcal{G}|}\sum_k R^{(k)}\vec{K} \\ &= i\hbar\,\frac{1}{|\mathcal{G}|}\sum_k\sum_{\alpha\beta}\mathrm{Im}[\chi_{\alpha,0}]R^{(k)}_{\alpha\beta}K_\beta \\ &= i\hbar\,\mathrm{Im}(\tilde{\vec{\chi}})\cdot\vec{K}\equiv\tilde{S}, \end{aligned} \tag{20}$$

where the new, BB-modified ''Hamiltonian'' $\tilde{S}$ is described by the new, rotated coordinate vector

$$\mathrm{Im}(\tilde{\vec{\chi}}) = \mathrm{Im}(\vec{\chi})\frac{1}{|\mathcal{G}|}\sum_k R^{(k)}. \tag{21}$$

Now, let the ideal, or ''wanted Hamiltonian'' be described by the coordinate vector $\vec{\chi}_w$, i.e.,

$$S_w = i\hbar\,\mathrm{Im}(\vec{\chi}_w)\cdot\vec{K}. \tag{22}$$

For storage this would correspond to the null vector, but not for computation. The goal of the empirical BB procedure is to find rotation matrices $R^{(k)}$ such that the difference

$$\tilde{S}-S_w = i\hbar[\mathrm{Im}(\tilde{\vec{\chi}})-\mathrm{Im}(\vec{\chi}_w)]\cdot\vec{K}=0, \tag{23}$$

or more generally, is minimal. This has the simple geometric interpretation of minimization of the distance between the BB-modified vector $\mathrm{Im}(\tilde{\vec{\chi}})$ and the desired vector $\mathrm{Im}(\vec{\chi}_w)$.

The *input data* is $\mathrm{Im}(\vec{\chi})$ (the output of the QPT measurement), $\vec{\chi}_w$ (the desired Hamiltonian), $\vec{K}$ (the operator basis, with respect to which $\vec{\chi}_w$ and $\vec{\chi}$ are defined). This data specifies a solution to Eqs. (21) and (23) in terms of the rotation matrices $R^{(k)}$. This solution is not unique; see, e.g., the example in Sec. V A.

When the $R^{(k)}$ are found, the BB pulses can be calculated from the transformation connecting the adjoint representation to its unitary group.

Thus Eqs. (21) and (23) can be viewed as the essence of the empirical BB procedure. From here on we flesh out this first main result.

B. Qubit noise

The development in Sec. III A was cavalier in its treatment of the indices α,β of the fixed operator basis $\{K_\alpha\}$. To be more precise, consider a quantum register of N qubits. We will derive a short-time expansion of Eq. (17) under the assumption that the system-bath interaction is linear in the system operators:

$$H^{(1)}_{SB} = \sum_{i=1}^{N}\vec{\sigma}_i\cdot\vec{B}_i, \tag{24}$$

where $\vec{\sigma}_i=(\sigma_i^x,\sigma_i^y,\sigma_i^z)$ is the vector of Pauli matrices acting on the ith qubit, and $\vec{B}_i$ is a corresponding vector of bath operators. This assumption will be relaxed below (Sec. III F) and, as should be clear from Sec. III A, is not essential for our approach, but will make the calculations below more transparent. A Taylor expansion of the evolution operator $U(t)$ [Eq. (1)] then reveals that as time increases, higher and higher tensor powers of the Pauli matrices act on the qubits

$$U(t) = I - itH^{(1)}_{SB} + \frac{(iH^{(1)}_{SB})^2}{2!}t^2+\cdots, \tag{25}$$

where for simplicity we have assumed a time-independent Hamiltonian and set $H_S=H_B=0$. The $O(t)$ term involves only single Pauli matrices, but the $O(t^2)$ terms and higher involve tensor products of Pauli matrices. To capture this in terms of the OSR we expand the fixed basis operators K_α as

$$K_{\vec{\alpha}_n} \equiv \bigotimes_{i=1}^{N}\sigma_i^\alpha, \tag{26}$$

where, for the ith qubit, σ_i^α, $\alpha=0,1,2,3$ corresponds to $I_i,\sigma_i^x,\sigma_i^y,\sigma_i^z$, respectively. The subscript on $K_{\vec{\alpha}_n}$ denotes a vector $\vec{\alpha}_n=(\alpha_1,\ldots,\alpha_N)$ with n nonzero entries. That is, $K_{\vec{\alpha}_n}$ acts nontrivially on n qubits. (We also use $\vec{\alpha}$ for a vector of arbitrary index.) Note that we have omitted the subscript i on α in Eq. (26) in order to reduce the index clutter. There exist $M=4^N$ different $K_{\vec{\alpha}_n}$ operators with $K_{\vec{\alpha}_0}=I\otimes\cdots\otimes I$ being the identity on the space of all qubits. Here we have chosen the K's to be Hermitian, and trace orthogonal,

$$\mathrm{Tr}(K_{\vec{\alpha}_m}K_{\vec{\beta}_n}) = 2^N\delta_{\vec{\alpha}_m\vec{\beta}_n}. \tag{27}$$

Hence they are a valid basis for all $2^N\times 2^N$ matrices.

Corresponding to this expansion of the fixed-basis operators, we can rewrite the OSR, Eq. (4), more explicitly as

$$\rho(t)=\sum_{m,n=0}^{N}\sum_{\vec{\alpha}_m,\vec{\beta}_n}\chi_{\vec{\alpha}_m,\vec{\beta}_n}(t)K_{\vec{\alpha}_m}\rho(0)K_{\vec{\beta}_n}$$
$$=\chi_{\vec{\alpha}_0,\vec{\beta}_0}(t)\rho(0)+\sum_{m=1}^{N}\sum_{\vec{\alpha}_m}\chi_{\vec{\alpha}_m,\vec{\beta}_0}(t)K_{\vec{\alpha}_m}\rho(0)$$
$$+\chi^{*}_{\vec{\alpha}_m,\vec{\beta}_0}(t)\rho(0)K^{\dagger}_{\vec{\alpha}_m}$$
$$+\sum_{m,n=1}^{N}\sum_{\vec{\alpha}_m,\vec{\beta}_n}\chi_{\vec{\alpha}_m,\vec{\beta}_n}(t)K_{\vec{\alpha}_m}\rho(0)K_{\vec{\beta}_n}. \quad (28)$$

Thus terms that contain only single Pauli matrices but not tensor products of Pauli matrices can only come from the second sum ($\Sigma_{m=1}^{N}\Sigma_{\vec{\alpha}_m}$), with $m=1$. Comparing to Eqs. (17) and (18) it is clear that this sum is responsible for (part of) the "Hamiltonian" $S(t)$, whereas the third sum generates the Lindblad-like term in Eq. (17). (This can also be verified directly by repeating the derivation in Refs. [47,60] using the $K_{\vec{\alpha}_n}$.) Hence to first order in t we find

$$\rho(t)-\rho(0)\approx -i[S(t),\rho(0)]$$
$$\approx t\left[\sum_{\vec{\alpha}_1}(\chi_{\vec{\alpha}_1,0}K_{\vec{\alpha}_1}-\chi^{*}_{\vec{\alpha}_1,0}K^{\dagger}_{\vec{\alpha}_1}),\rho(0)\right]$$
$$=-t\left[\sum_{\vec{\alpha}_1}\mathrm{Im}(\chi_{\vec{\alpha}_1,0})K_{\vec{\alpha}_1},\rho(0)\right], \quad (29)$$

where in the last line we used the Hermiticity of the K operators. The term $\Sigma_{\vec{\alpha}_1}$ is a sum over all elements of the Pauli group with one nonidentity element in the tensor product. By comparing to Eq. (25), and recalling the expression for the Kraus operators, Eq. (5), it follows that this term is directly related to bath matrix elements of H_{SB}, which give rise to a Lamb shift [47,60]. When the system Hamiltonian is included, it appears in the $\Sigma_{\vec{\alpha}_1}$ term as well. However, recall that we are developing an approach that is explicitly *model independent*. Hence the only quantities we will use are the QPT-measurable $\chi_{\vec{\alpha}_1,0}$.

We now wish to find an appropriate set of BB controls in order to eliminate the noise on our qubits. It should be clear from the discussion above that this noise is initially [i.e., at times of $O(t)$] produced by *unitary errors* associated with the bath-induced Lamb shift. Decoherence arises from terms that are of order $O(t^2)$. Decoherence suppression is achieved on a finite time scale with corrections being of order $O(\Delta t/\tau_c)^{2k}$ for a kth-order decoupling scheme, where Δt is the pulse interval and τ_c is the bath correlation time [16]. As noted above, from Secs. II A and II B we find that, under the action of BB controls, the K transform as

$$K_{\vec{\alpha}}\overset{\mathrm{BB}}{\rightarrow}\frac{1}{|\mathcal{G}|}\sum_k U_k^{\dagger}K_{\vec{\alpha}}U_k. \quad (30)$$

(Here $\vec{\alpha}$ denotes a vector of arbitrary index.) This transformation is the basis for much of what follows.

C. Qubit storage

For the storage of information (without computation) in qubits, we need to preserve the density matrix under time evolution, so that $\rho(t)=\rho(0)$. Let us denote BB-modified quantities by a tilde. In this case we should have, using Eq. (29),

$$[\tilde{S}(t),\rho(0)]=0 \quad (31)$$

as the BB control objective. Since S does not contain an identity component I we require that

$$\tilde{S}(t)=0. \quad (32)$$

We proceed to turn this into a condition on BB pulses.

Recall that $K_{\vec{\alpha}_1}$ denotes an operator with exactly one nonidentity term (one of the three Pauli matrices acting on an unspecified qubit). There are therefore $3N$ such operators, which we now denote explicitly as σ_i^{α}, where $i=1,\ldots,N$, and $\alpha=1,2,3$. Under the assumption of a linear system-bath coupling, Eq. (24), it is clear that the BB pulses need only involve tensor products of single-qubit unitaries, i.e.,

$$U_k=\bigotimes_{i=1}^{N}U_i^{(k)}.$$

Then Eq. (30) becomes

$$\sigma_i^{\alpha}\overset{\mathrm{BB}}{\rightarrow}\frac{1}{|\mathcal{G}|}\sum_k U_k^{\dagger}\sigma_i^{\alpha}U_k$$
$$=\frac{1}{|\mathcal{G}|}\sum_k U_i^{(k)\dagger}\sigma_i^{\alpha}U_i^{(k)}. \quad (33)$$

At this point it is useful to again introduce real rotation matrices R to represent the BB group,

$$U_i^{(k)\dagger}\sigma_i^{\alpha}U_i^{(k)}=\sum_{\beta=1}^{3}R^{i;(k)}_{\alpha\beta}\sigma_i^{\beta}. \quad (34)$$

Here i runs over qubit indices; $k\in\{0,1,\ldots,|\mathcal{G}|-1\}$; $R^{i;(k)}$ is in the adjoint representation of the group SU(2) [i.e., $R^{i;(k)}\in\mathrm{SO}(3)$] acting on the ith qubit and has matrix elements $R^{i;(k)}_{\alpha\beta}$. Now let us consider the transformation of $S(t)$ under the BB controls. To simplify notation let us denote

$$\xi^i_{\alpha}\equiv\mathrm{Im}(\chi^i_{\alpha,0}). \quad (35)$$

Then from Eq. (29)

$$\frac{i}{t}S(t)\approx\sum_i\sum_{\alpha}\xi^i_{\alpha}\sigma_i^{\alpha}\equiv\sum_i\vec{\xi}^i\cdot\vec{\sigma}_i, \quad (36)$$

$$\frac{i}{t}S(t)\overset{\mathrm{BB}}{\rightarrow}\sum_i\vec{\xi}^{\,i}\cdot\frac{1}{|\mathcal{G}|}\sum_k U_i^{(k)\dagger}\vec{\sigma}_iU_i^{(k)}$$
$$=\sum_i\vec{\xi}^{\,i}\cdot\frac{1}{|\mathcal{G}|}\sum_k R^{i;(k)}\cdot\vec{\sigma}_i$$
$$=\sum_i\vec{\tilde{\xi}}^{\,i}\cdot\vec{\sigma}_i, \quad (37)$$

where

$$\left(\frac{1}{|\mathcal{G}|}\sum_k R^{i;(k)}\right)\vec{\xi}^i=\vec{\tilde{\xi}}^i. \tag{38}$$

For storage we require $\vec{\tilde{\xi}}^i=0$, i.e.,

$$\tilde{\xi}^i_\beta=\mathrm{Im}(\tilde{\chi}^i_{\beta,0})=0 \quad \forall\ \beta,i. \tag{39}$$

Thus, *solving for each i the set of linear equations*

$$\sum_k\sum_\alpha \mathrm{Im}(\chi^i_{\alpha,0})R^{i;(k)}_{\alpha\beta}=0 \tag{40}$$

for the rotation matrix elements $R^{i;(k)}$, *in terms of measurable parameters* $\chi^i_{\alpha,0}$ (*the output of a* QPT *experiment*), *determines the BB pulses empirically*. The pulse form of the BB controls is determined through Eq. (34).

Note that if $\mathrm{Im}(\chi^i_{\alpha,0})\equiv\mathrm{Im}(\chi_{\alpha,0})$, i.e., there is no dependence on qubit index (collective decoherence [6,9]), then the same set of rotation matrices $\{R^{(k)}\}_{k=0}^{|\mathcal{G}|-1}$ (with matrix elements $R^{(k)}_{\alpha\beta}$) can be used for all qubits, as already pointed out in Ref. [16] in terms of unitary BB controls. It also shows that, for complete symmetrization, one need only ensure that $\Sigma_k R^{i;(k)}_{\alpha\beta}=0$ for all α,β, independent of the decoherence mechanism.

Finally, note that we can rewrite Eq. (40) as

$$\left(\frac{1}{|\mathcal{G}|}\sum_k R^{i;(k)}\right)\mathrm{Im}(\vec{\chi}^i)=0. \tag{41}$$

In this manner it is clear that what we are looking for is a group of rotation matrices $\{R^{i;(k)}\}$, acting on qubit *i*, whose average $(1/|\mathcal{G}|)\Sigma_k R^{i;(k)}$ acts to annihilate the QPT measurement output vector $\mathrm{Im}(\vec{\chi}^i)$. This is the geometrical interpretation of the empirical BB condition. Equation (41) is our second main result.

D. Single-qubit operations

Now suppose that we are interested in quantum *computation*. In this case we must allow for single- and two-qubit operations, such that these are not eliminated by the BB controls. In the model-dependent approach this translates into the (sufficient) condition that the BB generators commute with the Hamiltonian that is implementing the computation [17,18]. Here we derive more general conditions from the empirical BB perspective, which have the advantage that they can be used to determine the required set of BB pulses directly from a QPT measurement and a stipulated, wanted system Hamiltonian.

Let us consider the case of single-qubit operations first. In this case the system Hamiltonian need only contain a single nonidentity operator (Pauli matrix) per qubit, as in Eq. (24). Therefore, the development of the previous subsection applies. The difference, however, is that now instead of the storage condition of Eq. (39), we require the BB-modified χ-matrix elements $\tilde{\chi}^i_{\beta,0}$ to assume values that correspond to a *wanted* evolution (or system Hamiltonian S_w). Let us denote the corresponding wanted (real) χ-matrix elements by w^i_β (they can easily be calculated from a Hamiltonian—see below); then the empirical BB condition replacing Eq. (40) becomes

$$\frac{1}{|\mathcal{G}|}\sum_k\sum_\alpha \mathrm{Im}(\chi^i_{\alpha,0})R^{i;(k)}_{\alpha\beta}=w^i_\beta. \tag{42}$$

This once again has to be solved for the rotation matrices $R^{i;(k)}$, with elements $R^{i;(k)}_{\alpha\beta}$, given the empirical data $\vec{\tilde{\chi}}^i \equiv\mathrm{Im}(\tilde{\chi}^i_{\alpha,0})$. This too, can be written in a form amenable to a geometric interpretation

$$\left(\frac{1}{|\mathcal{G}|}\sum_k R^{i;(k)}\right)\mathrm{Im}(\vec{\chi}^i)=\vec{w}^i. \tag{43}$$

Now the average over the rotation matrices acts to rotate the QPT output vector to a desired vector for the *i*th qubit $\vec{w}^i$. Equation (43) is our third main result.

E. Solvability

Let us next discuss the solvability conditions for the rotation matrices $R^{i;(k)}$, from Eqs. (41) and (43). Since the vanishing of $(1/|\mathcal{G}|)\Sigma_k R^{i;(k)}$ suffices to satisfy Eq. (41) for given *i*, its solvability is guaranteed if the $R^{i;(k)}$ are chosen such that, given *i*, the $R^{i;(k)}$ correspond to *transformations onto the vertices of a symmetric object in three dimensions*. We stress that this is only a sufficient condition, which yields a solution that is independent of the empirical data $\vec{\chi}^i$. One can also solve Eq. (41) for the rotation matrices $R^{i;(k)}$ such that $\vec{\chi}^i$ lies in the kernel of the linear transformation $\Sigma_k R^{i;(k)}$. This is a standard linear algebra problem. The condition for a nonempty kernel is the vanishing of the determinant of the linear transformation. The dimension of the kernel is the number of linearly independent vectors that are annihilated by the linear transformation. Since we require that Eq. (41) be satisfied for all qubits *i*, it is clear that sometimes the kernel space can be too small. However, given the great deal of flexibility in choosing the rotation matrices, it seems that in practice a solution can always be found, even if one insists on not having $\Sigma_k R^{i;(k)}\equiv 0$.

As for Eq. (43), this is just the inhomogeneous version of the linear algebra problem discussed above, and similar standard arguments apply. However, some more insight into a sufficient condition may be obtained through a geometric argument, as follows. Let us focus on the case of a single qubit (thus dropping the index *i*), and denote $\vec{w}=(a,b,c)^t$, $\mathrm{Im}(\chi_{\alpha,0})=(d,e,f)^t$. We can always find a rotation matrix T such that

$$T\begin{pmatrix}a\\ b\\ c\end{pmatrix}=\begin{pmatrix}a'\\ 0\\ 0\end{pmatrix}. \tag{44}$$

Then $(d,e,f)^t\rightarrow(d',e',f')^t$ under T, and we can write Eq. (43) as

$$T\left(\frac{1}{|\mathcal{G}|}\sum_k R^{(k)}\right)T^{-1}\begin{pmatrix} d' \\ e' \\ f' \end{pmatrix}=\begin{pmatrix} a' \\ 0 \\ 0 \end{pmatrix}. \tag{45}$$

Then in the rotated frame, we may write

$$T\left(\frac{1}{|\mathcal{G}|}\sum_k R^{(k)}\right)T^{-1}=\begin{pmatrix} \sum_k q^{(k)} \\ \\ \sum_k M^{(k)} \end{pmatrix},$$

such that the BB rotations have an upper 1×3 row that should solve the equation $\Sigma_k q^{(k)}d'=a'$, and a lower 2×3 block that is the sum of 2×3 matrices $\Sigma_k M^{(k)}$ that should vanish. That is, the $M^{(k)}$ correspond to *transformations onto the vertices of a symmetric object in the plane orthogonal to the "a′ direction."* The generalization to more than one qubit is straightforward.

For both Eqs. (41) and (43) we stipulate that our available BB rotations have these properties. If not, we use the results of Sec. IV to encode our information into a subspace such that these conditions are indeed satisfied.

F. Two-qubit operations

In order to implement two-qubit operations we must allow for a system Hamiltonian that contains two-body interactions. Therefore, it is useful to comment on what happens when also the system-bath Hamiltonian contains higher-order coupling, e.g., second order

$$H_{SB}^{(2)}=\sum_{j>i=1}^{N}(\vec{\sigma}_i\cdot G_{ij}\cdot\vec{\sigma}_j)\otimes B_{ij}, \tag{46}$$

where G_{ij} is a second-rank tensor. In this case, both the third and fourth line of Eq. (28) contribute terms that are bilinear in the Pauli matrices, i.e., they contribute $\Sigma_{\vec{\alpha}_2}$ and $\Sigma_{\vec{\alpha}_1,\vec{\beta}_1}$, respectively. Additional bilinear terms will arise when the expansion is taken to $O(t^2)$. The latter may arise from $H_{SB}^{(1)}$ [Eq. (24)] and will contribute to the *nonunitary, decohering* part of the evolution. The BB pulses that are appropriate for all these cases will be elements of SU(4).

As before, the quantities extracted from the QPT measurements will be the imaginary part of the χ matrix which we abbreviate using a matrix ξ, as in Eq. (35). In this case the modified evolution will provide for the possibility of two-qubit interactions. Thus, generalizing from Eqs. (29) and (36),

$$\frac{i}{t}S(t)\approx\left[\sum_{\vec{\alpha}_2}\mathrm{Im}(\chi_{\vec{\alpha}_2,0})K_{\vec{\alpha}_2}+\sum_{\vec{\alpha}_1}\mathrm{Im}(\chi_{\vec{\alpha}_1})K_{\vec{\alpha}_1},\rho(0)\right]$$
$$=\sum_{ij}\vec{\sigma}_i\cdot\overleftrightarrow{\xi}^{ij}\cdot\vec{\sigma}_j, \tag{47}$$

where

$$(\xi^{ij})_{\alpha\beta}=\xi_{\alpha\beta}^{ij}\equiv\mathrm{Im}(\chi_{\alpha\beta,00}^{ij})+\mathrm{Im}(\chi_{\alpha 0,00}^{ij}) \tag{48}$$

is a 4×4 matrix of coefficients. Under the action of the set of BB controls,

$$\frac{i}{t}S(t)\overset{\mathrm{BB}}{\rightarrow}\frac{1}{|\mathcal{G}|}\sum_k\sum_{ij}U_{ij}^{(k)\dagger}(\vec{\sigma}_i\cdot\overleftrightarrow{\xi}^{ij}\cdot\vec{\sigma}_j)U_{ij}^{(k)}$$
$$=\sum_{ij}\vec{\sigma}_i\cdot\overleftrightarrow{\tilde{\xi}}^{ij}\cdot\vec{\sigma}_j, \tag{49}$$

where

$$\overleftrightarrow{\tilde{\xi}}^{ij}=\frac{1}{|\mathcal{G}|}\sum_k R^{ij;(k)}\cdot\overleftrightarrow{\xi}^{ij}, \tag{50}$$

and the rotation matrices $R\in\mathrm{SO}(15)$ are defined through

$$U_{ij}^{(k)\dagger}(\sigma_i^\alpha\otimes\sigma_j^\beta)U_{ij}^{(k)}=\sum_{\gamma\delta}R_{\alpha\beta,\gamma\delta}^{ij;(k)}(\sigma_i^\gamma\otimes\sigma_j^\delta). \tag{51}$$

Again, let us describe the target, or wanted, evolution by the χ-matrix w. In analogy with Eq. (34), the matrix R is in the adjoint representation of the group and thus can be viewed as a rotation in the vector space of Hermitian matrices. In this case, only a subgroup of the rotation group SO(N) is represented by the adjoint action. (This is true for all SU(n), $n\geqslant 3$). The expression analogous to Eq. (43) becomes

$$\frac{1}{|\mathcal{G}|}\sum_k R^{ij;(k)}\cdot\overleftrightarrow{\xi}^{ij}=\overleftrightarrow{w}_{ij}, \tag{52}$$

or using explicit index notation,

$$\frac{1}{|\mathcal{G}|}\sum_k\sum_{\gamma\delta}\xi_{\gamma\delta}^{ij}R_{\gamma\delta,\alpha\beta}^{ij;(k)}=w_{\alpha\beta}^{ij}. \tag{53}$$

Thus the two-qubit case involves solving for the elements of each of the rotation matrices $R^{ij;(k)}$, given the QPT data $\overleftrightarrow{\xi}^{ij}$ and the desired Hamiltonian $\overleftrightarrow{w}_{ij}$. After the rotation matrices are found, one obtains the BB pulses by inverting Eq. (51) for the $U_{ij}^{(k)}$. While this seems like a daunting task in general, it should be numerically tractable, and is illustrated for a simple example in Sec. V B below. Equation (52) is our fourth main result.

IV. GENERALIZATION TO ENCODED QUBITS

Before presenting examples, we generalize the empirical BB condition to encoded qubits, such as arise in the theory of quantum error correcting codes (QECC) [2–5] and decoherence-free subspaces (DFS) [6–11]. In both cases it is highly desirable to let the experiment determine a "tailored encoding," since the experiment knows the decoherence processes that govern the system we wish to protect better than any model one can design. Furthermore, combining QECC and DFS with the BB method has proven to be a powerful tool [25–28,61]. Now, both QECC and DFS can be described in terms of a *stabilizer* [5,10]. A stabilizer group for a set of code words, i.e., a code space, is a subgroup (of the Pauli group for QECC, and of the group of all unitary transformations for DFS) that leaves the code space invariant. A

code (whether QECC or DFS) can be completely specified in terms of its stabilizer [62].

Let $\mathcal{S}$ be the vector space (group algebra) generated by real linear combinations of the set of generators of the stabilizer group. Any member of $\mathcal{S}$ will leave the code space invariant. Thus the most general ''error'' we can allow in the outcome of a BB procedure, when compared to a given wanted Hamiltonian, is an error in $\mathcal{S}$. Then the outcome of this ''erroneous'' evolution will be correct up to an overall phase. As before, let $\mathrm{Im}(\vec{w})$ be the coordinates of the vector corresponding to the desired Hamiltonian evolution and $\mathrm{Im}(\vec{\tilde{\chi}})$ be the actual vector after BB operations. Formally, the condition is

$$\tilde{S}-S_w=i\hbar[\mathrm{Im}(\vec{\tilde{\chi}})-\mathrm{Im}(\vec{w})]\cdot\vec{K}\in\mathcal{S}, \tag{54}$$

which should be compared to Eq. (23). This equation may be interpreted in either of two ways. First, given an encoding and a wanted Hamiltonian S_w, it can be solved for the BB operations that are needed for the suppression of errors on the code subspace. Second, given a physically implementable set of BB operations, it can be solved for a compatible code (by finding the stabilizer). Abstractly, this procedure may be seen as a projection of the open system evolution onto an evolution which is in the stabilizer of the code space. The geometric projection operation completely reduces to the group-theoretical projection onto the commutant given in Ref. [15] in the case that the set of $R^{(k)}$, form a discrete group [24]. The emphasis here is a geometric picture of the empirical operations projecting onto the stabilizer group of the code. Note that quite generally, Eq. (54) *gives an empirical means of identifying a subspace encoding such that the BB operations drive the evolution into a subspace which does not affect the encoded states*. This implies a general, empirical means for the *creation of a* DFS [27]. Equation (54) is our fifth main result, which is new and quite general.

If the BB procedure is imperfect there will be an error component remaining. The error vector $\vec{E}$ is given by the difference between the BB modified and wanted Hamiltonians in the (n^2-1)-dimensional vector space, where our geometric picture holds

$$\vec{E}=\mathrm{Im}(\vec{\tilde{\chi}})-\mathrm{Im}(\vec{w}). \tag{55}$$

The vector $\vec{E}$ gives the magnitude and direction of the error (i.e., the basis elements λ_i give the type of error, e.g., bit flip and/or phase flip, etc.). The corresponding scalar quantity (distance) is

$$d(\mathrm{Im}\vec{\tilde{\chi}},\mathrm{Im}(\vec{w}))=[\mathrm{Tr}(\mathrm{Im}(\vec{\tilde{\chi}})-\mathrm{Im}(\vec{w}))^2]^{1/2}. \tag{56}$$

The error (55) can be generalized to

$$d(\mathcal{S},\mathrm{Im}(\vec{\tilde{\chi}}))=\min_{\vec{B}\in\mathcal{S}}[\vec{B}-\mathrm{Im}(\vec{\tilde{\chi}})], \tag{57}$$

and likewise, the corresponding scalar quantity is

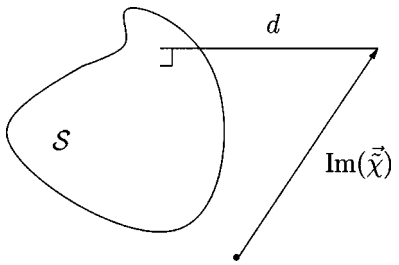

FIG. 1. Visualization of the error d that remains after the application of BB pulses. $\mathrm{Im}(\vec{\tilde{\chi}})$ is the BB-modified coordinate vector of the evolution, and d measures the distance to the closest element of the algebra of the stabilizer group of the code.

$$d(\mathcal{S},\mathrm{Im}(\vec{\tilde{\chi}}))=\min_{\vec{B}\in\mathcal{S}}[\mathrm{Tr}(\vec{B}-\mathrm{Im}(\vec{\tilde{\chi}}))^2]^{1/2}, \tag{58}$$

which can be visualized as in Fig. 1.

Similar conclusions were presented for the unencoded case in Ref. [24].

V. EXAMPLES

In this section we study several examples that illustrate the formalism developed above.

A. One-qubit example: Storing a qubit in the presence of pure dephasing

Let us consider a simple model: a phase-flip error (pure dephasing) on a single qubit. To first order, this gives a density matrix of the form

$$\rho_s'\approx\rho_s+\left(\frac{igt}{2}\right)[\rho_s,\sigma_z], \tag{59}$$

where the prime indicates the density matrix for the qubit after the interaction with a bath. The coupling constant g is a measure of the strength of the interaction. The bath time scale is the inverse of the bath high-frequency cutoff, which is a separate parameter. Suppose that we wish to find a set of BB pulses that *store* this qubit.

The first step in the empirical BB procedure is to measure the superoperator using QPT. Here we would discover that the interaction causes a phase-flip error which corresponds to $K\propto\sigma_z$. That is, a measurement of the χ matrix would yield [by the comparison of Eq. (59) to Eq. (29)]: $\{\mathrm{Im}(\chi^1_{\alpha,0})\}_{\alpha=x,y,z}=\{0,0,-g/2\}$.

The next step is to find the optimal set of BB operations. This we can do by solving Eq. (41) for the rotation matrices with the measured χ matrix. This yields

$$-\frac{g}{2}\left(\sum_{k=0}^{|\mathcal{G}|-1}R^{(k)}_{3\beta}\right)=0 \quad\Rightarrow\quad \sum_{k=0}^{|\mathcal{G}|-1}R^{(k)}_{3\beta}=0. \tag{60}$$

In accordance with the BB operations forming a discrete subgroup, $k=0$ corresponds to the identity. For $n=1$, since $R_{31}=0$ for the identity rotation,

$$0+\sum_{k=1}^{|\mathcal{G}|-1}R^{(k)}_{3\beta}=0 \quad\text{and}\quad 1+\sum_{k=1}^{|\mathcal{G}|-1}R^{(k)}_{33}=0, \tag{61}$$

where $\beta=1,2$.

The best set of BB operations is the set that accomplishes the task at hand and has the fewest elements $|\mathcal{G}|$. We now find a set with $|\mathcal{G}|=2$ (corresponding to a parity-kick solution [12,14]). That is, we seek a rotation matrix

$$R^{(1)}=\begin{pmatrix} & & 0 \\ & & 0 \\ 0 & 0 & -1 \end{pmatrix},$$

whose unspecified elements are arbitrary in as far as that they do not affect the outcome of the BB procedure. To transform from the rotation matrices back to the BB pulses [i.e., from SO(3) back to SU(2)], we use the general result

$$\begin{aligned}(R\cdot\vec{\sigma})_\alpha &= e^{i\hat{n}\cdot\vec{\sigma}\theta}\sigma_\alpha e^{-i\hat{n}\cdot\vec{\sigma}\theta} \\ &= \sigma_\alpha\cos(2\theta)+2n_\alpha(\hat{n}\cdot\vec{\sigma})\sin^2(\theta) \\ &\quad -(\hat{n}\times\vec{\sigma})_\alpha\sin(2\theta). \end{aligned} \tag{62}$$

Here $R\in\mathrm{SO}(3)$, $\hat{n}$ is a unit vector along the axis in $\mathbb{R}^3$ about which a rotation through an angle θ is performed [these 4 parameters parametrize the SO(3) rotation matrices]. Let $\alpha=3$, then we know from the form of $R^{(1)}$ that

$$-\sigma_z=\sigma_z\cos(2\theta)+2n_3(\hat{n}\cdot\vec{\sigma})\sin^2(\theta)-(\hat{n}\times\vec{\sigma})_z\sin(2\theta).$$

It is simple to check that (mod 2π) the unique solution to this equation is $\theta=\pm\pi/2$, $n_3=0$. This implies $U=e^{\pm i\hat{n}\cdot\vec{\sigma}\pi/2}$, with $\hat{n}=(n_1,n_2,0)$, but otherwise arbitrary. The BB pulse must therefore correspond to a rotation about a unit vector in the $x-y$ plane on the Bloch sphere, which is the expected result as the error was along the z axis.

It is likely that in a real experiment pure dephasing will not be the only source of decoherence. Let us consider a situation where this was the dominant source, so that our QPT measurement that yielded $\{\mathrm{Im}(\chi^1_{\alpha;0})\}_{\alpha=x,y,z}=\{0,0,-g/2\}$ actually contained an x component as well, which was too small to be noticed while the dephasing process was present, e.g., because the two errors may well have different characteristic time scales. Suppose that we perform another QPT measurement while applying the BB pulses found above (that eliminated dephasing) and find a residual error of the σ_x (bit-flip) type. This is an instance of a learning loop, which we discuss in Sec. VI below.

In this case, consider the total Hamiltonian

$$H=\frac{g'}{2}\sigma_x\otimes(I+\sigma_x). \tag{63}$$

Proceeding in exactly the same manner as before we determine the required BB operations. We find that we need to implement $U=e^{\pm\hat{n}\cdot\vec{\sigma}\pi/2}$, where now $\hat{n}=(0,n_2,n_3)$. Combining this and the condition $\hat{n}=(n_1,n_2,0)$, we find that we need to use $\hat{n}=(0,n_2,0)$. Thus bit and phase flips might be corrected using the corresponding single BB operation, which would be determined empirically from an experiment with a learning-loop process. This is an optimal set, since it will eliminate both errors with only one (nonidentity) BB pulse per cycle.

B. Two-qubit example: Computation using the Heisenberg interaction in the presence of independent dephasing

As indicated above, the problem in the two-qubit case can be quite involved since, in general, it requires finding the elements of rotation matrices in SO(15). To illustrate the formalism we consider a simple example. Suppose we wish to implement a Heisenberg exchange interaction $J\vec{\sigma}_1\cdot\vec{\sigma}_2$ between the two qubits (Heisenberg exchange is important in a number of promising solid-state proposals, and is an interaction that is all by itself universal for QC [10,29,62]). Then the wanted, Heisenberg interaction is determined from

$$H_{\mathrm{Heis}}=J\vec{\sigma}_1\cdot\vec{\sigma}_2=\sum_{ij}\sum_{\alpha\beta}\sigma_i^\alpha w_{\alpha\beta}^{ij}\sigma_j^\beta,$$

so that it is described by the matrix

$$\overleftrightarrow{w}_{12}=J\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}. \tag{64}$$

Further, suppose that our QPT measurements suggest that the source of decoherence in the experiment is independent dephasing on the two qubits. This will be detected through QPT by producing the following:

$$\frac{i}{t}S(t)\approx g_1\sigma_1^z+g_2\sigma_2^z=\sum_{ij}\sum_{\alpha\beta}\sigma_i^\alpha\xi_{\alpha\beta}^{ij}\sigma_j^\beta. \tag{65}$$

Independent dephasing will thus be described by the matrix elements

$$\xi^{12}_{3,0}=g_1,\qquad \xi^{12}_{0,3}=g_2. \tag{66}$$

To find the set of BB pulses we would now need to solve Eq. (53) for the rotation matrix elements, and then determine the corresponding SU(4) transformations, in a manner analogous to what we did above in the single-qubit example. As noted above (see also Ref. [24]), solving these equations is not, in general, trivial. In this simple example, however, a set of BB controls can be found noting the trace orthogonality of the two algebraic basis elements [24], those corresponding to the exchange and those corresponding to the errors. Rather than going through a full derivation, we present the solution. To remove the independent dephasing through a parity-kick procedure, without affecting the Heisenberg exchange interaction, it is possible to use independent qubit interactions which form the following pulse:

$$U\equiv U_1U_2=\exp[-i(\sigma_1^x+\sigma_2^x)\pi/2]=-\sigma_1^x\sigma_2^x. \tag{67}$$

By direct calculation one can show that

$$[U,H_{\mathrm{Heis}}]=0\quad\text{and}\quad\{U,S\}=0. \tag{68}$$

The first commutation relation ensures that the parity-kick pulse can be applied during the computation with H_{Heis}, while the second (anti)commutation relation is the parity-kick condition [12,14,24]. Thus the desired evolution is achieved. The pulse U is certainly not unique, and a general solution of Eq. (52) would yield a variety of other possible pulses.

VI. OPTIMIZATION ALGORITHMS

As indicated in the single-qubit example discussed in the preceding section, the empirical BB procedure can benefit from the incorporation of an off-line learning loop, that acts as an optimization algorithm for the BB pulses. Such learning loops have proven very successful, e.g., in quantum-chemical applications, where they are typically used to optimize the yield of a chemical reaction, steer a system towards a desired state, or perform a cooling task [37–43]. Roughly, the idea is to guide a quantum system toward a desired goal by letting a learning algorithm optimize a classical control field (e.g., a laser pulse). An initial field is guessed and applied to the quantum system. The output is measured and input into a search algorithm (e.g., a genetic algorithm [41,63]), which tries to optimize the field in order to get closer to the desired goal. The experiment is then repeated with the new field, and the process is repeated until it converges to the desired goal to within a prescribed tolerance.

A. Variational optimization

We first present an outline of a variational optimization procedure, which can, in principle, be used to tailor our BB pulses. Our presentation follows the standard approach in the quantum control literature, e.g., Refs. [38,39]. The general control problem can be stated as follows. We seek a system Hamiltonian, H_c, which modifies a given (total, system-bath) Hamiltonian H, so as to produce the desired effective Hamiltonian

$$\tilde{H}=H+H_c. \tag{69}$$

The control Hamiltonian H_c may be composed of several possible terms,

$$H_c=\sum_i u_i(t)H_c^i, \tag{70}$$

where the $u_i(t)$ are usually pulses in QC, analogous to the control fields in NMR and quantum optical systems. That is, the $u_i(t)$ are control fields that may be turned on and off as desired. The unitary evolution will proceed as usual according to $U(t)=\mathcal{T}\exp[-i\int^t\tilde{H}(t')dt']$ with H, H_c acting simultaneously. Thus controllability is determined by the group space that one is able to generate by the exponentiated vector fields $\tilde{H}$ [64]. For the robust storage of a qubit using BB controls, we require the elimination of the interaction Hamiltonian H. This would correspond to have $U\approx I$. We also wish to use as few BB operations as possible due to the time constraints. Thus we seek to minimize the difference between the BB-modified Hamiltonian $\tilde{S}$, and the desired Hamiltonian S_w

$$\Delta S\equiv\tilde{S}-S_w, \tag{71}$$

where $\tilde{S}$ and S_w are the appropriate modifications to Eq. (18). For example, for storage we would want $S_w=0$. One may now consider the standard controllability problem in terms of a desired state of the system, to be reached from some initial state $|a_0\rangle\equiv|a(t=0)\rangle$:

$$i|\dot{a}(t)\rangle=\tilde{H}|a(t)\rangle \tag{72}$$

(formally we should have included bath states as well, but we omit these for notational convenience). $\tilde{H}=\tilde{H}(u_i(t),t)$ and we may formally write the solution as

$$\begin{aligned}|a(t)\rangle&=U(t,t_0)|a_0\rangle\\&=\left[\mathcal{T}\exp\left\{\int_{t_0}^t\tilde{H}(u_i(\tau),\tau)d\tau\right\}\right]|a_0\rangle.\end{aligned} \tag{73}$$

This can be seen as essentially a Heisenberg picture control problem [16] and one can thus eliminate the direct inclusion of the state itself. The short-time approximation enables us to remove the time ordering and write the expanded form

$$U(t,t_0)=\lim_{\Delta t_k\to 0}[\exp\{-i\tilde{H}_{N-1}\Delta t_{N-1}\}\cdots\exp\{-i\tilde{H}_0\Delta t_0\}]. \tag{74}$$

At this point we may invoke the assumptions of the BB operations that they are short, strong pulses and the evolution in between them be that of the free system and bath.

It should be pointed out that in the standard control theory one often uses the *final state* as the target of the control. This can be done as a variational procedure, or in conjunction with numerical algorithms which drive a learning or real-time feedback loop. However, in quantum information processing applications, it is often the *evolution itself* that is the control target, rather than the final state. For example, one would like to optimize the noiselessness of the evolution, as in our case. This fundamental difference between the goals of traditional control theory and its potential application in the quantum information domain has yet to be explored. An interesting recent step in this direction was taken in Refs. [65,66], in the context of optimization of *unitary* (closed-system) evolutions.

To optimize the BB procedure, the difference between the BB modified controls and the ideal evolution should be minimized. This may be achieved in the continuum by solving the variational problem with a variable end point. The appropriate variational problem can be formulated as the minimization of a *cost function* J [38–43], expressed in terms of the control fields $\{u_i\}$ and cycle time T_c as

$$J=\int_{t_0}^{MT_c}(\mathrm{Tr}\{[S(u(\tau),\tau)-S_w(\tau)]^2\})^{1/2}d\tau, \tag{75}$$

where $a^2 \equiv a^\dagger a$ and we have used M cycle times T_c for the end point (which is not fixed). One may add experimental constraints, such as finite pulse energy, smoothness of the pulse shapes, etc. [38,39]. This is a standard variational problem for which we would seek $\delta J = 0$ and $\delta^2 J < 0$. The outcome, i.e., the solution to the variational problem, will be the optimal control fields $\{u_i\}$. Note that these fields will be approximately continuous for large M and small Δt. Then we may approximate them by a discrete set of BB operations (traditionally defined as piecewise continuous controls; see, e.g., Refs. [64,67]). However, it is to be expected that one of the advantages of the optimization procedure is that it will yield pulses that are easier to implement physically than the pulses coming out of a standard BB analysis, since the optimization procedure can be formulated to explicitly take into account experimental constraints. In fact, experience in quantum chemistry shows that the pulses found by an optimization procedure are often highly nonintuitive [38–43].

Questions of convergence, etc., can be avoided by the use of a subgroup with a small number of elements. This will reduce the problem, under the BB assumptions, to a search on a discrete space. This is the space of discrete, or finite order, subgroups of unitary groups. Fortunately, for quantum computation, we require only one- and two-qubit operations which reduces our search spaces to those of the discrete subgroups of SU(2) and/or SU(4). These have been classified (see Refs. [68–70] and references therein). We will not pursue the variational formulation further here. An actual variational optimization calculation will be presented in a future publication.

B. Learning algorithm

In certain cases it may be possible to perform a large number of experiments on identically prepared samples, differing in the applied control fields. In this case, instead of solving a variational problem to find optimal BB pulses, one can try to let the experiment guide an off-line learning algorithm (typically a genetic algorithm) to an optimal solution [41]. This algorithm is a part of a learning loop, described in Fig. 2.

The learning loop consists of the following steps, which are repeated iteratively in the learning process.

(1) A quantum state is *input* for a particular information processing task.

(2) The state is allowed to interact with a bath and undergo noisy evolution in the *experiment*. Here we may choose to apply BB pulses to modify the evolution.

(3) The resulting evolution is obtained through *quantum process tomography*.

(4) The QPT data is *analyzed* by the learning algorithm to find an improved BB strategy. This involves solving key Eqs. (43) and (52).

(5) The previous steps are repeated until convergence to within a prescribed tolerance is attained.

The result of the procedure is an optimized set of BB pulses. This set includes (i) the least number of BB operations that will reduce or eliminate the noise in the system, and (ii) the optimal ordering for this minimal set.

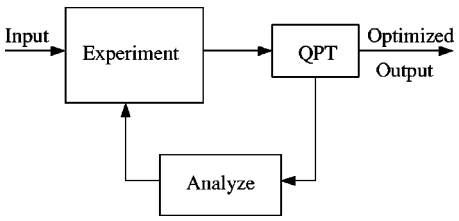

FIG. 2. The learning loop control diagram for the empirical determination of the optimal bang-bang controls.

Let us emphasize that: (1) no knowledge of the total Hamiltonian or noise process is assumed (i.e., the optimal implementation is determined empirically), and (2) no assumption is made about the quality of the BB operations, only that they should improve the fidelity of the desired operations. (Of course we know from earlier work [12–19] that the BB operations should be implemented as strong fast pulses, but imperfect implementation will still reduce noise.)

Finally, let us note that the learning process could, in principle, be incorporated in a real-time feedback loop (e.g., Ref. [71] and references therein), but this would require a very fast numerical algorithm to solve Eqs. (43) and (52).

VII. CONCLUDING REMARKS

In order for methods that reduce decoherence and noise in quantum information processing tasks to succeed in the real world, they must be confronted with experimental data, and allowed to be optimized in response to this data. This is the approach we have taken here, in the context of the dynamical decoupling, or ''bang-bang'' (BB) method. We have developed a formulation of the BB method that allows one to *tailor* the BB control pulses in response to data acquired by a quantum process tomography experiment. The experiment supplies a set of numbers that characterize the noise processes occurring on a short-time scale. From these numbers one can determine an optimal set of BB pulses, by solving a set of linear equations, in particular, Eqs. (23), (41), (43), and (52). These equations correspond to different tasks one may wish to implement with the help of the BB pulses (respectively, general storage, single-qubit storage, single-qubit computation, two-qubit computation), and yield a set of rotation matrices (R) that correspond to BB pulses that perform the desired tasks.

A promising generalization of a single-shot tomography-BB experiment is to introduce an off-line learning loop, that uses the above equations in order to determine an optimized set of BB pulses. The learning process incorporates tomography measurements from a previous round in order to find improved BB pulses for the next round. We have briefly discussed how such a loop, and a concomitant variational optimization procedure, can be designed.

Throughout this paper we have emphasized that our results have an intuitive interpretation in terms of a geometric picture, wherein the effect of BB pulses is to rotate a coordinate vector representing a noisy Hamiltonian to a desired

Hamiltonian. The geometric picture, via Eq. (54), also enables the determination of the ability to create an encoding (such as a decoherence-free subspace) using empirical data and the available set of BB pulses. Alternatively, it can be used to describe the appropriate set of BB operations required to eliminate noise from an encoded set of qubits.

We hope that the results presented here will stimulate experiments in which real data will drive the determination and application of appropriately tailored BB pulses.

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