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Control of inhomogeneous quantum ensembles

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Finding control fields (pulse sequences) that can compensate for the dispersion in the parameters governing the evolution of a quantum system is an important problem in coherent spectroscopy and quantum information processing. The use of composite pulses for compensating dispersion in system dynamics is widely known and applied. In this paper, we make explicit the key aspects of the dynamics that makes such a compensation possible. We highlight the role of Lie algebras and noncommutativity in the design of a compensating pulse sequence. Finally, we investigate three common dispersions in NMR spectroscopy, namely the Larmor dispersion, rf inhomogeneity, and strength of couplings between the spins.

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Many applications in control of quantum systems involve controlling a large ensemble by using the same control field. In practice, the elements of the ensemble could show variation in the parameters that govern the dynamics of the system. For example, in magnetic resonance experiments, the spins of an ensemble may have large dispersion in their natural frequencies (Larmor dispersion), strength of applied rf field (rf inhomogeneity), and the relaxation rates of the spins [1]. In solid-state NMR spectroscopy of powders, the random distribution of orientations of internuclear vectors of coupled spins within an ensemble leads to a distribution of coupling strengths [12]. A canonical problem in control of quantum ensembles is to develop external excitations that can simultaneously steer the ensemble of systems with variation in their internal parameters from an initial state to a desired final state. These are called compensating pulse sequences as they can compensate for the dispersion in the system dynamics. From the standpoint of mathematical control theory, the challenge is to simultaneously steer a continuum of systems between points of interest with the same control signal. Typical applications are the design of excitation and inversion pulses in NMR spectroscopy in the presence of Larmor dispersion and rf inhomogeneity [1–10] or the transfer of coherence or polarization in a coupled spin ensemble with variations in the coupling strengths [13]. In many cases of practical interest, one wants to find a control field that prepares the final state as some desired function of the parameter, for example slice selective excitation and inversion pulses in magnetic resonance imaging [14–17]. The problem of designing excitations that can compensate for dispersion in the dynamics is a well studied subject in NMR spectroscopy, and extensive literature exists on the subject of composite pulses that correct for dispersion in system dynamics [1–7]. Composite pulses have recently been used in quantum information processing to correct for systematic errors in single- and two-qubit operations [18–23]. The focus of this paper is not to construct a new compensating pulse sequence but rather to highlight the aspects of system dynamics that make such a compensation possible and give proofs of the existence of a compensating pulse sequence. Our final goal is to develop a better understanding of what kind of dispersions can and cannot be corrected.

To fix ideas, consider an ensemble of noninteracting spin $\frac{1}{2}$ in a static field B_0 along z axis and a transverse rf field, $(A(t)\cos\phi(t), A(t)\sin\phi(t))$, in the x-y plane. The dispersion in the amplitude of the rf field is captured by a dispersion parameter ϵ such that $A(t)=\epsilon A_0(t)$, where $\epsilon\in[1-\delta,1+\delta]$, for $\delta>0$. Similarly dispersion in B_0 leads to a spread in the Larmor frequency $\omega=\gamma B_0$ (γ is the gyromagnetic ratio of the spins) around a nominal value ω_0, i.e., $\omega-\omega_0=\Delta\omega\in[-B,B]$. Let x,y,z represent the coordinates of the unit vector in direction of the net magnetization vector of the ensemble. The Bloch equations for the ensemble take the form

$$\frac{d}{dt}\begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 0 & -\omega & \epsilon u(t) \\ \omega & 0 & -\epsilon v(t) \\ -\epsilon u(t) & \epsilon v(t) & 0 \end{bmatrix}\begin{bmatrix} x \\ y \\ z \end{bmatrix}, \tag{1}$$

where $u(t)=\gamma A_0(t)\cos\phi(t)$ and $v(t)=\gamma A_0(t)\sin\phi(t)$. Let $X(t)$ denote the unit vector $[x(t),y(t),z(t)]$. Consider now the problem of designing controls $u(t)$ and $v(t)$ that simultaneously steer an ensemble of such systems with dispersion in their natural frequency and strength of rf field from an initial state $X(0)=(0,0,1)$ to a final state $X_F=(1,0,0)$ [8]. This problem raises interesting questions about controllability, i.e., showing that in spite of bounds on the strength of rf field, $\sqrt{u^2(t)+v^2(t)}\leq A_{\max}$, there exist excitations $(u(t),v(t))$ that simultaneously steer all the systems with dispersion in ω and ϵ, to a ball of desired radius r around the final state $(1,0,0)$ in a finite time (which may depend on $A_{\max}$, B, δ, and r). Besides steering the ensemble between two points, we can ask for a control field that steers an initial distribution of the ensemble to a final distribution, i.e., different elements of the ensemble now have different initial and final states depending on the value of their parameters (ω,ϵ). The initial and final state of the ensemble is described by functions $X_0(\omega,\epsilon)$ and $X_F(\omega,\epsilon)$, respectively. Consider the problem of steering an initial distribution $X_0(\omega,\epsilon)$ to within a desired distance r of a target function $X_F(\omega,\epsilon)$ by appropriate choice of controls in Eq. (1) (distance between two functions refers to the standard L_2 distance). If a system with dispersion in parameters can be steered between states that have depen-

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dency on the dispersion parameter, then we say that the system is ensemble-controllable with respect to these parameters.

This paper is organized as follows. First, we introduce the key ideas and, through examples, highlight the role of Lie brackets and noncommutativity in the design of a compensating control. Next, we study ensemble controllability of the Bloch equations (1) in the presence of Larmor dispersion and rf inhomogeneity with bounded controls, $u(t)$ and $v(t)$. We conclude the paper with some observations on time-varying dispersions and questions related to optimal control of inhomogeneous ensembles.

Example 1: Main concept. To fix ideas, we begin by considering Bloch equations $\dot{X}=\epsilon[u(t)\Omega_y+v(t)\Omega_x]X$ in a rotating frame with only rf inhomogeneity and no Larmor dispersion, where

$$\Omega_x=\begin{bmatrix}0&0&0\\0&0&-1\\0&1&0\end{bmatrix},\quad \Omega_y=\begin{bmatrix}0&0&1\\0&0&0\\-1&0&0\end{bmatrix},\quad \Omega_z=\begin{bmatrix}0&-1&0\\1&0&0\\0&0&0\end{bmatrix}$$

are the generators of rotation around the x, y, and z axis, respectively. Observe for small dt, the evolution $U_1(dt)=\exp(-\epsilon\Omega_y\sqrt{dt})\exp(-\epsilon\Omega_x\sqrt{dt})\exp(\epsilon\Omega_y\sqrt{dt})\exp(\epsilon\Omega_x\sqrt{dt})$ to leading order in dt is given by $\mathbf{1}+(dt)[\epsilon\Omega_y,\epsilon\Omega_x]$, i.e., we can synthesize the generator $[\epsilon\Omega_x,\epsilon\Omega_y]=\epsilon^2\Omega_z$, by back and forth maneuver in the directly accessible directions Ω_x and Ω_y.

Similarly, the leading-order term in the evolution $U_2=\exp(-\epsilon\Omega_y dt)U_1(-\sqrt{dt})\exp(\epsilon\Omega_y dt)U_1(\sqrt{dt})$ is $ad^2_{\epsilon\Omega_y}(\epsilon\Omega_x)=[\epsilon\Omega_y,[\epsilon\Omega_y,\epsilon\Omega_x]]=-\epsilon^3\Omega_x$. Therefore, by successive Lie brackets, we can synthesize terms of the type $\epsilon^{2k+1}\Omega_x$. Now using $\{\epsilon\Omega_x,\epsilon^3\Omega_x,\ldots,\epsilon^{2n+1}\Omega_x\}$ as generators, we can produce an evolution $\exp\{\Sigma_{k=0}^{n}c_k\epsilon^{2k+1}\Omega_x\}$, where n and the coefficients c_k can be chosen so that $\Sigma_{k=0}^{n}c_k\epsilon^{2k+1}\approx\theta$ for all $\epsilon\in[1-\delta,1+\delta]$. Hence we can generate an evolution $\exp(\theta\Omega_x)$ for all ϵ to any desired accuracy. Therefore, we achieve robustness with dispersion to ϵ by generating suitable Lie brackets. Similar arguments show that we can generate any evolution $\exp(\beta\Omega_y)$ and as a result any three-dimensional rotation in a robust way. It is also now easy to see that we can synthesize rotation Θ with a desired functional dependency on the parameter ϵ. Parametrize a rotation in $\Theta\in SO(3)$ by the Euler angles (α,β,γ) such that $\Theta=\exp(\alpha\Omega_x)\exp(\beta\Omega_y)\exp(\gamma\Omega_x)$. Given functions $(\alpha(\epsilon),\beta(\epsilon),\gamma(\epsilon))$ of ϵ, we can find polynomials that approximate $\alpha(\epsilon)$, $\beta(\epsilon)$, and $\gamma(\epsilon)$ arbitrarily well and use these to generate a desired rotation $\Theta(\epsilon)$ as a function of ϵ. Hence there exists a control field that maps a smooth initial distribution $X_0(\epsilon)$ to a target distribution $X_F(\epsilon)$.

Remark: Note we have assumed that $\epsilon>0$. The above system will fail to be ensemble-controllable if $\epsilon\in[-\epsilon_0,\epsilon_0]$, as we cannot approximate an even function $f(\epsilon)=\theta$ with an odd degree polynomial.

Remark: Complexity of implementation. The key idea in designing a compensating pulse sequence is to synthesize higher-order Lie brackets that raise the dispersion parameters to higher powers. The various powers of the dispersion parameter can be combined for compensation, as explained above. We now analyze the time complexity of generating higher-order Lie brackets. The propagator $U_{k+1}(dt)=\exp(-\epsilon\Omega_y\sqrt{dt})U_k(-\sqrt{dt})\exp(\epsilon\Omega_y\sqrt{dt})U_k(\sqrt{dt})$ to leading order is $\mathbf{1}+\epsilon^{k+1}ad^{k+1}_{\Omega_y}\Omega_x dt$, where $U_0(dt)=\exp(\epsilon\Omega_x dt)$. Let $T_{k+1}(dt)$ be the time required to produce the propagator $U_{k+1}(dt)$, then $T_{k+1}(dt)=2[\sqrt{dt}+T_k(\sqrt{dt})]$, with $T_0(dt)=dt$. This then gives that $T_k(dt)$ scales as $2^k dt^{1/2^k}$. Therefore, synthesizing higher-order brackets is expensive. For example, for $dt=10^{-4}$, synthesis of $U_2(dt)\approx\mathbf{1}+\epsilon^3\Omega_x dt$ takes of the order of $dt^{1/4}=0.1$ units of time, which is 10^3 times longer than the evolution $\exp(-\epsilon\Omega_x dt)$. Thus the construction presented here is not the most efficient way of achieving a desired level of compensation, however it depicts in a transparent way the role of higher-order Lie bracketing.

Example 2: Phase dispersions cannot be compensated. Consider an ensemble of Bloch equations

$$\dot{X}_\theta=A(t)\{\cos[\phi(t)+\theta]\Omega_x+\sin[\phi(t)+\theta]\Omega_y\}X_\theta, \qquad (2)$$

where there is a dispersion in the phase of the rf field. The system is not ensemble-controllable with respect to the dispersion $\theta\in[\theta_1,\theta_2]$.

Proof: The simplest way to see this is to make the change of coordinates $Y_\theta=\exp(-\Omega_z\theta)X_\theta$. The resulting system then takes the form $\dot{Y}_\theta=A(t)\{\cos[\phi(t)]\Omega_x+\sin[\phi(t)]\Omega_y\}Y_\theta$. Since all Y_θ see the same field, they have identical trajectories. As a result, X_θ cannot be simultaneously steered from $(0,0,1)$ to $(1,0,0)$. The lack of ensemble controllability can also be understood by looking at Lie brackets of the generators. Equation (2) can be written as $\dot{X}_\theta=\{A(t)\cos[\phi(t)]B_1+A(t)\sin[\phi(t)]B_2\}X_\theta$, where the $B_1=\cos(\theta)\Omega_x+\sin(\theta)\Omega_y$ and $B_2=-\sin(\theta)\Omega_x+\cos(\theta)\Omega_y$. Observe that $B_3=[B_1,B_2]=\Omega_z$. Therefore, all iterated brackets of $B_i's$ are linear in $\cos(\theta)$ and $\sin(\theta)$ and we cannot raise the dispersion parameters $\cos(\theta)$ and $\sin(\theta)$ to higher powers and therefore cannot compensate for the dispersion in θ.

Example 3: Larmor dispersion in the presence of strong rf field. Now consider the Bloch equations $\dot{X}_\theta=[\omega\Omega_z+u(t)\Omega_x+v(t)\Omega_y]X_\theta$ with dispersion in the Larmor frequencies. The system is ensemble-controllable with respect to the dispersion parameter ω.

Note because of the assumption of strong fields, we can reverse the evolution of the drift term

$$\exp(\pi\Omega_x)\exp(\omega\Omega_z dt)\exp(-\pi\Omega_x)=\exp(-\omega\Omega_z dt). \qquad (3)$$

Now as before, a maneuver $\exp(-\omega\Omega_z\sqrt{dt})\exp(-\Omega_x\sqrt{dt})\times\exp(\omega\Omega_z\sqrt{dt})\exp(\Omega_x\sqrt{dt})$ produces the bracket direction $[\omega\Omega_z,\Omega_x]=\omega\Omega_y$ to leading order. Similarly $ad^2_{(\omega\Omega_z)}\Omega_x=[\omega\Omega_z[\omega\Omega_z,\Omega_x]]=-(\omega)^2\Omega_x$. Hence, we can generate higher brackets with even and odd powers of ω. To see that the system is ensemble-controllable, consider the Lie bracket relation $ad^{2n}_{(\omega\Omega_z)}\Omega_x=(-1)^n\omega^{2n}\Omega_x$ and $ad^{2n+1}_{(\omega\Omega_z)}\Omega_y=(-1)^{n+1}\omega^{2n+1}\Omega_x$. We can synthesize an evolution $\exp(\Sigma_k c_k\omega^k\Omega_x)$ and similarly the evolution $\exp(\Sigma_k d_k\omega^k\Omega_y)$. The coefficients c_k and d_k can be chosen to approximate

Euler angles $(\alpha(\omega),\beta(\omega),\gamma(\omega))$, and as in Example 1, they have ensemble controllability.

Example 4: Dispersion in coupling strengths. Consider two coupled qubits with Ising-type interactions with dispersion in coupling strengths J. The interaction Hamiltonian $H_c=J\sigma_{1z}\sigma_{2z}$, with $J\in J_0[1-\delta,1+\delta]$, $\delta>0$. Although not necessary, for simplicity of exposition, we assume that we can produce local unitary transformation on the qubits much faster than the evolution of couplings. We now show that it is possible to compensate for dispersion in J and generate any quantum logic with high fidelity.

By local transformations we can synthesize the effective Hamiltonian $J\sigma_{1y}\sigma_{2z}=\exp(i\sigma_{1x}\pi/2)(J\sigma_{1z}\sigma_{2z})\exp(-i\sigma_{1x}\pi/2)$. Now using $B_1=-i2\sigma_{1y}\sigma_{2z}$ and $B_2=-i2\sigma_{1z}\sigma_{2z}$ as generators, we get $[JB_1[JB_1,JB_2]]=-J^3B_2$. Now using a construction similar to the one in Example 1, we can synthesize the evolution $\exp(\Sigma_k c_k J^{2k+1}\sigma_{1z}\sigma_{2z})$, where the coefficients c_k are chosen such that $\Sigma_k c_k J^{2k+1}\approx J_0$ over the range of dispersion of J. Hence we have to compensate for dispersion in J. We also have ensemble controllability with respect to the parameter J. We can choose coefficients c_k to approximate a smooth function of J and hence synthesize $A(J)=\exp\{-i[a(J)\sigma_{1x}\sigma_{2x}+b(J)\sigma_{1y}\sigma_{2y}+c(J)\sigma_{1z}\sigma_{2z}]\}$. We can write an arbitrary two-qubit gate with the dependency on J as $U_2(J)\otimes U_1(J)A(J)V_2(J)\otimes V_1(J)$, where U_1,V_1 and U_2,V_2 are local unitaries on qubits 1 and 2, respectively. We can synthesize them with an explicit dependence on J as follows. Using the commutation relations of the type $[-iJ2\sigma_{1y}\sigma_{1z},-iJ2\sigma_{1z}\sigma_{1z}]=-iJ^2\sigma_{1x}$, we can synthesize generators $-i(J^2)^k\sigma_{1x}$, $-i(J^2)^k\sigma_{1y}$, $-i(J^2)^k\sigma_{2x}$, $-i(J^2)^k\sigma_{2y}$ $(k=0,1,2,\ldots)$ and use these to synthesize $U_1(J),V_1(J),U_2(J),V_2(J)$.

Remark: Using ideas similar to those above, it is possible to compensate for dispersion in a more general coupling tensor. Consider the coupling tensor $\alpha\sigma_{1x}\sigma_{2x}+\beta\sigma_{1y}\sigma_{2y}+\gamma\sigma_{1z}\sigma_{2z}$ with dispersion in α,β,γ. Now observe for $U=\exp(-i\pi\sigma_z)$ and $A=\exp[-i(\alpha\sigma_{1x}\sigma_{2x}+\beta\sigma_{1y}\sigma_{2y}+\gamma\sigma_{1z}\sigma_{2z})]$, $UAU^{\dagger}A=\exp(-i\gamma 2\sigma_{1z}\sigma_{2z})$. So we only need to take care of the dispersion in γ, and the construction is similar to the one before.

We consider again the system (1) but now with bounded controls, so that we cannot produce rotations of the type $\exp(-\Omega_x\pi)$ in arbitrarily small time as in Eq. (3). Nonetheless, the system is ensemble-controllable as shown below. To begin with, assume there is no dispersion in the rf-field amplitude. Our construction initially follows the well known algorithm of Shinnar-Roux [16,17]. We then show how this construction can be extended to show ensemble controllability with respect to Larmor dispersion and rf inhomogeneity in Bloch equations. The solution to the Bloch equation (1) is a rotation $X(T)=RX(0)$, where $R\in\mathrm{SO}(3)$. We work with SU(2) representation of these rotations, where a rotation by angle ϕ around the unit vector (n_x,n_y,n_z) has a representation of the form $U=\left[\begin{smallmatrix}\alpha & -\beta^*\\ \beta & \alpha^*\end{smallmatrix}\right]$, where α and β are the Cayley-Klein parameters satisfying $\alpha=\cos(\phi/2)-in_z\sin(\phi/2)$, $\beta=-i(n_x+in_y)\sin(\phi/2)$, and $\alpha\alpha^*+\beta\beta^*=1$. The Bloch equation then takes the form

$$\dot{U}=-\frac{i}{2}\begin{bmatrix}\omega & u-iv\\ u+iv & -\omega\end{bmatrix}U.$$

The rotation U is simply represented by its first column (also termed spinor representation) $\psi=\left[\begin{smallmatrix}\alpha\\ \beta\end{smallmatrix}\right]$. We first consider piecewise-constant controls $u(t)$ and $v(t)$. The net rotation under these controls can be represented as successive rotations $U=U_nU_{n-1}\cdots U_1U_0$, where $U_j=\left[\begin{smallmatrix}a_j & -b_j^*\\ b_j & a_j^*\end{smallmatrix}\right]$ and a_j,b_j are the Cayley-Klein parameters for the jth interval. Defining the multiplication of the matrices U_j up to k by

$$\begin{bmatrix}\alpha_k & -\beta_k^*\\ \beta_k & \alpha_k^*\end{bmatrix}=\begin{bmatrix}a_k & -b_k^*\\ b_k & a_k^*\end{bmatrix}\cdots\begin{bmatrix}a_0 & -b_0^*\\ b_0 & a_0^*\end{bmatrix},$$

the effect of the controls can then be calculated by propagating the spinor

$$\begin{bmatrix}\alpha_k\\ \beta_k\end{bmatrix}=\begin{bmatrix}a_k & -b_k^*\\ b_k & a_k^*\end{bmatrix}\begin{bmatrix}\alpha_{k-1}\\ \beta_{k-1}\end{bmatrix}\tag{4}$$

with the initial condition $\left[\begin{smallmatrix}\alpha_0\\ \beta_0\end{smallmatrix}\right]=\left[\begin{smallmatrix}1\\ 0\end{smallmatrix}\right]$. The duration Δt, over which the controls u and v are constant, can be chosen small enough such that the net rotation can be decomposed into two sequential rotations since $e^{(\omega\Omega_z+u\Omega_y-v\Omega_x)\Delta t}\approx e^{(u\Omega_y-v\Omega_x)\Delta t}e^{\omega\Omega_z\Delta t}$. Under this assumption, we can write the rotation U_k as a rotation around the z axis by an angle $\omega\Delta t$ followed by a rotation about the applied control fields by an angle ϕ_k in SU(2) representation,

$$U_k=\begin{bmatrix}C_k & -S_k^*\\ S_k & C_k\end{bmatrix}\begin{bmatrix}z^{1/2} & 0\\ 0 & z^{-1/2}\end{bmatrix},\tag{5}$$

where

$$C_k=\cos\phi_k/2,\quad S_k=-ie^{i\theta_k}\sin\phi_k/2,\quad \phi_k=A_k\Delta t,$$
$$\theta_k=\tan^{-1}v_k/u_k,\quad A_k=\sqrt{u_k^2+v_k^2},\quad z=e^{-i\omega\Delta t}.\tag{6}$$

Plugging Eq. (5) into Eq. (4), we get the recursion relation of the spinor,

$$\begin{bmatrix}\alpha_k\\ \beta_k\end{bmatrix}=z^{1/2}\begin{bmatrix}C_k & -S_k^*z^{-1}\\ S_k & C_kz^{-1}\end{bmatrix}\begin{bmatrix}\alpha_{k-1}\\ \beta_{k-1}\end{bmatrix}.$$

Defining $P_k=z^{-k/2}\alpha_k$ and $Q_k=z^{-k/2}\beta_k$, the recursion may then be reduced to

$$\begin{bmatrix}P_k\\ Q_k\end{bmatrix}=\begin{bmatrix}C_k & -S_k^*z^{-1}\\ S_k & C_kz^{-1}\end{bmatrix}\begin{bmatrix}P_{k-1}\\ Q_{k-1}\end{bmatrix}\tag{7}$$

with the initial condition

$$\begin{bmatrix}P_0\\ Q_0\end{bmatrix}=\begin{bmatrix}1\\ 0\end{bmatrix}.\tag{8}$$

From the recursion (7) and the initial condition (8), the spinor at the nth time step can be represented as the $(n-1)$-order polynomials in z, $P_n(z)=\Sigma_{k=0}^{n-1}p_kz^{-k}$, and $Q_n(z)=\Sigma_{k=0}^{n-1}q_kz^{-k}$ where $|P_n(z)|^2+|Q_n(z)|^2=1$ [the parameter $p_0=\Pi_{k=1}^{n}\cos(\phi_k/2)$]. The parameter z encodes the dispersion parameter ω. The desired final states of an ensemble of systems in Eq. (1), described by Cayley-Klein parameters, are two functions of z, and hence of ω. We can now design two polynomials $P_n(z)$ and $Q_n(z)$ such that we can approximate any desired smooth functions $F_\alpha(z)$ and $F_\beta(z)$ satisfying $|F_\alpha(z)|^2+|F_\beta(z)|^2=1$, which characterizes the desired spinor we want as a function of z. Now we can work backwards and compute the u_k's and v_k's that will produce $P_n(z)$ and $Q_n(z)$.

Note that by multiplying both sides of Eq. (7) by the inverse of the rotation matrix, we get

$$\begin{bmatrix} P_{k-1} \\ Q_{k-1} \end{bmatrix} = \begin{bmatrix} C_k P_k + S_k^* Q_k \\ (-S_k P_k + C_k Q_k) z \end{bmatrix}. \tag{9}$$

We have a backward recursion where we use the knowledge of coefficients of $P_k(z)$ and $Q_k(z)$ to compute $P_{k-1}(z)$ and $Q_{k-1}(z)$ [16,17] algorithm. Because $P_{k-1}(z)$ and $Q_{k-1}(z)$ are lower-order polynomials, the leading term in $P_{k-1}(z)$ and the low-order term in $Q_{k-1}(z)$ must drop out,

$$C_k P_{k,k-1} + S_k^* Q_{k,k-1} = 0, \tag{10}$$

$$-S_k P_{k,0} + C_k Q_{k,0} = 0, \tag{11}$$

where $P_{k,m}$ denotes the coefficient of z^{-m} term in $P_k(z)$. These two equations are equivalent. Choosing Eq. (11) and combining it with Eq. (7), we get $Q_{k,0}/P_{k,0} = -ie^{i\theta_k}\tan(\phi_k/2)$. This gives the flip angle $\phi_k = 2\tan^{-1}|Q_{k,0}/P_{k,0}|$ and the phase $\theta_k = \sphericalangle(iQ_{k,0}/P_{k,0})$. The controls are then $u_k = (\phi_k/\Delta t)\sin\theta_k$, and $v_k = (\phi_k/\Delta t)\cos\theta_k$. These expressions for controls coupled with the inverse recursion in Eq. (9) construct the piecewise constant controls u_k, v_k that generate polynomial approximations $P_n(z)$ and $Q_n(z)$ of the target function $F_\alpha(z)$ and $F_\beta(z)$.

In particular, if we choose $\beta_n(z) = z^{n/2} Q_n(z) \approx -i\sin(\phi/2)$ and $\alpha_n(z) = z^{n/2} P_n(z) \approx \cos(\phi/2)$, we obtain a broadband rotation (uniform over all ω) around the x axis by angle ϕ, and similarly by choosing $\beta_n(z) = \sin(\phi/2)$ and $\alpha_n(z) = \cos(\phi/2)$, we obtain an approximation to a broadband rotation around the y axis by angle ϕ.

Now we consider the case when there is also rf inhomogeneity. We again write the final rotation $U \in SU(2)$ as $U = U_n U_{n-1} \cdots U_1 U_0$, where

$$U_k(z,\epsilon) = \begin{bmatrix} C_k(\epsilon) & -S_k(\epsilon)^* \\ S_k(\epsilon) & C_k(\epsilon) \end{bmatrix} \begin{bmatrix} z^{1/2} & 0 \\ 0 & z^{-1/2} \end{bmatrix}.$$

Note that the flip angle has a dependence on the parameter ϵ, and for small flip angles ϕ_k we have

$$\begin{bmatrix} C_k(\epsilon) & -S_k^*(\epsilon) \\ S_k(\epsilon) & C_k(\epsilon) \end{bmatrix} = \begin{bmatrix} 1-(\phi_k\epsilon)^2/8 & -ie^{-i\theta_k}\phi_k\epsilon/2 \\ -ie^{i\theta_k}\phi_k\epsilon/2 & 1-(\phi_k\epsilon)^2/8 \end{bmatrix}.$$

This results in the polynomials $P_z(z,\epsilon) = \Sigma_{k=0}^{n-1} p_k(\epsilon) z^{-k}$ and $Q_n(z,\epsilon) = \Sigma_{k=0}^{n-1} q_k(\epsilon) z^{-k}$ in Eq. (7). These polynomials can be used to approximate a desired response as a function of ω and ϵ. Such constructions can also be used to generate pattern pulses that selectively excite the Bloch equations with parameters lying in a given subset of ω-ϵ space [10].

In this paper, we have tried to make explicit the role of noncommutativity as a key aspect of the dynamics that makes design of a compensating control possible. We introduced the method of polynomial approximations for design of pulse sequences for controlling inhomogeneous quantum ensembles. We note again that the constructions given in this paper do not provide the most efficient schemes for compensation; however, the constructions presented here establish the existence of a compensating pulse sequence in a transparent manner. Finding efficient compensating pulse sequences is a problem in optimal control. In our recent work, we demonstrated how simple gradient descent algorithms [11] can be used to search for efficient compensation schemes. These algorithms have recently been applied for the design of broadband excitation and inversion pulses in the presence of rf inhomogeneity [9,10].

In this paper, we have assumed that the dispersion in the parameters of the Hamiltonian are stationary. Another class of problems of both fundamental and practical interest are design of excitations that are insensitive to random fluctuations in the parameters of the Hamiltonian. For example, there has been recent interest in the design of high-fidelity single-qubit gates in the presence of random telegraph noise (RTN) [24]. The noise is characterized by random fluctuations in ω in the Bloch Eq. (1), such that ω is a random process that jumps between $-\Delta$ and Δ with a correlation time t_c, so that the probability density of interarrival time t between two jumps is $\exp(-t/t_c)$. The goal is to design an excitation for steering Eq. (1) that is immune to such fluctuations [24]. Further work is required to understand the controllability of such problems.

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