Noncommuting vector fields, polynomial approximations and 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 non-commutativity in the design of a compensating pulse sequence. Finally we investigate three common dispersions in NMR spectroscopy, the Larmor dispersion, rf-inhomogeneity and strength of couplings between the spins.

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I. INTRODUCTION

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. In solid state NMR spectroscopy of powders, the random distribution of orientations of inter-nuclear vectors of coupled spins within an ensemble leads to a distribution of coupling strengths. 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 or the transfer of coherence or polarization in coupled spin ensemble with variations in the coupling strengths. 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. 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. 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 existence of a compensating pulse sequence. Our final goal is to understand what kind of dispersions can and cannot be corrected.

To fix ideas, consider an ensemble of noninteracting spin 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. Let $x, y, z$ represent the coordinates of the unit vector in direction of the net magnetization vector of the ensemble. The dispersion in the amplitude of the rf-field is given by a dispersion parameter $\epsilon$ such that $A(t) = \epsilon_0(t)$ where $\epsilon \in [1-\delta, 1+\delta]$, for $\delta > 0$. Similarly there is dispersion in the larmor frequency $\omega$ around a nominal value $\omega_0$, i.e., $\omega - \omega_0 = \Delta \omega \in [-B, B]$. In a rotating frame rotating with frequency $\omega_0$, the Bloch equations take the form

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

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 $(x, y, z) = (0, 0, 1)$ to a final state $(x, y, z) = (1, 0, 0)$. This problem raises interesting questions about controllability, i.e., showing that inspite of bounds on the strength of rf-field, $\sqrt{u^2(t) + v^2(t)} \leq A_{max}$, there exist excitations $(u(t), v(t))$, which simultaneously steer all the systems with dispersion in $\Delta \omega$ and $\epsilon$, to a ball of desired radius $r$ around the final state $(1, 0, 0)$ in a finite time (which may depend on $A_{max}$, $B$, $\delta$, and $r$). These are control prob-
lems involving infinite dimensional systems with special structure. Besides steering the ensemble between two points, we can ask for a control that steers an initial distribution of the ensemble to a final distribution, i.e., if \( X(t) \) denote the units vector \( (x(t), y(t), z(t)) \), consider the problem of steering an initial distribution \( X(\Delta \omega, \epsilon, 0) \) to a target function \( X(\Delta \omega, \epsilon, T) \) by appropriate choice of controls in equation (11). If a system with dispersion in parameters can be steered between states that have dependency on the dispersion parameter, then we say that the system is ensemble controllable with respect to these parameters. A more formal definition will appear later in the paper.

This paper is organized as follows. In the following section, we introduce the key ideas and through examples, highlight the role of Lie brackets and non-commutativity in the design of a compensating control. In section 3, we show that the Bloch equations (11), with bounded controls, \( u(t) \) and \( v(t) \) are ensemble controllable in the presence of Larmor dispersion and rf-inhomogeneity. Finally in section 4, we investigate in some generality, the notion of ensemble controllability for linear control systems and a class of nonlinear control systems.

II. Lie Brackets and Ensemble Controllability

Example 1: Main Concept To fix ideas, we begin by considering Bloch equations with only rf-inhomogeneity and no Larmor dispersion.

\[
\dot{X} = \epsilon(u(t)\Omega_y + v(t)\Omega_x)X
\]

where

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

are the generators of rotation around \( x \), \( y \) and \( z \) axis, respectively.

Observe for small \( dt \), the evolution \( U_1(\sqrt{\epsilon}dt) = \exp(-\epsilon\Omega_y\sqrt{\epsilon}dt) \exp(-\epsilon\Omega_x\sqrt{\epsilon}dt) \exp(\epsilon\Omega_y\sqrt{\epsilon}dt) \exp(\epsilon\Omega_x\sqrt{\epsilon}dt) \)
to leading order in \( dt \) is given by \( I + (dt)[\epsilon\Omega_y, \epsilon\Omega_x] \), 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 \( \Omega_x \) and \( \Omega_y \).

Similarly, the leading order term in the evolution

\[
U_2 = U_1(-\sqrt{\epsilon}dt) \exp(-\epsilon\Omega_y dt)U_1(\sqrt{\epsilon}dt) \exp(\epsilon\Omega_y dt).
\]

is \( \epsilon\Omega_y, [\epsilon\Omega_x, \epsilon\Omega_y] = \epsilon^2\Omega_z \). Therefore by successive Lie brackets, we can synthesize terms of the type \( \epsilon^{2k+1}\Omega_z \). Now using \( \{\epsilon\Omega_x, \epsilon^2\Omega_z, \ldots, \epsilon^{2n+1}\Omega_z\} \) as generators, we can produce an evolution

\[
\exp\left\{\sum_{k=0}^{n} c_k \epsilon^{2k+1}\Omega_z\right\},
\]

where \( n \) and the coefficient \( c_k \) can be chosen so that

\[
\sum_{k=0}^{n} c_k \epsilon^{2k+1} \approx \theta
\]

for all \( \epsilon \in [1 - \delta, 1 + \delta] \). Hence we can generate an evolution \( \exp(\theta) \) for all \( \epsilon \) to any desired accuracy. Therefore, we achieve robustness with dispersion by generating suitable Lie brackets. Similar arguments show that we can generate any evolution \( \exp(\beta) \) and as a result any three dimensional rotation in a robust way. It is also now easy to see that we can synthesize rotation \( \Theta \) with a desired functional dependency on the parameter \( \epsilon \).

Parametrize a rotation in \( \Theta \in SO(3) \) by the Euler angles \((\alpha, \beta, \gamma)\) such that \( \Theta = \exp(\alpha \Omega_x) \exp(\beta \Omega_y) \exp(\gamma \Omega_z) \). Given continuous function \((\alpha(\epsilon), \beta(\epsilon), \gamma(\epsilon))\), of \( \epsilon \), 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 \( \epsilon \). Hence there exists a control field that maps a smooth initial distribution \( X_c(0) \) to a target distribution \( X_T^\theta \).

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 The key idea in designing 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. The construction presented here is not the most efficient way of achieving a desired level of compensation. The construction given here however presents in a transparent way the role of higher order lie bracketing. We now consider an example when there are more than one parameter in the system dynamics.

Example 2 Now consider the system

\[
\dot{X} = (\epsilon_1 u(t)\Omega_x + \epsilon_2 v(t)\Omega_y)X
\]

where \( \epsilon_1 \in [1 - \delta_1, 1 + \delta_1] \) and \( \epsilon_2 \in [1 - \delta_2, 1 + \delta_2] \), for \( 0 < \delta_1 < 1 \) and \( 0 < \delta_2 < 1 \). The system is ensemble controllable with respect to dispersions \( \epsilon_1 \) and \( \epsilon_2 \).

The reasoning proceeds along the same lines as before except now we have two dispersions parameters that are independent. Let \( ad^2_X(Y) \) represent the lie bracket \([X, Y]\) (similarly \( ad^2_Y(Y) = [X, [X, Y]] \)). Consider the identity,

\[
ad^2_{\epsilon_1\Omega_x}(\epsilon_2\Omega_y) = (-1)^k \epsilon_1^{2k+1} \epsilon_2 \Omega_z.
\]

for \( k = 0, 1, 2, \ldots, n \).

We can now choose coefficients \( c_k \) such that \( \sum_k c_k \epsilon^{2k+1} \) approximates a constant function over the range of \( \epsilon_1 \). As a result, we can generate the bracket direction \( \epsilon_2 \Omega_z \). Now using the bracket directions \( \epsilon_2 \Omega_z \) and \( \epsilon_2 \Omega_y \), and the construction in Example 1, we can further compensate the dispersion of \( \epsilon_2 \) and steer the whole ensemble together to a desired point. Infact the final point
can be made to depend explicitly on $\epsilon_1$ and $\epsilon_2$ by syn-
thesizing the bracket directions $\sum_k (c_k \epsilon_1 \epsilon_2^{2k+1}) \Omega_z$, and
$\sum_k (d_k \epsilon_1 \epsilon_2^{2k+1}) \Omega_y$. The coefficients $c_k$ and $d_k$
can be now so chosen that we can approximate rotations $\exp(\theta(\epsilon_1, \epsilon_2) \Omega_x)$ and $\exp(\theta(\epsilon_1, \epsilon_2) \Omega_y)$. Therefore we have
ensemble controllability.

**Example 3:** Phase dispersions cannot be com-
penated

Consider an ensemble of Bloch equations

$$\dot{X}_\theta = A(t)(\cos(\phi(t) + \theta) \Omega_x + \sin(\phi(t) + \theta) \Omega_y) X_\theta, \quad (3)$$

where there is 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 co-ordinates $Y_\theta = \exp(-\Omega_z \theta) X_\theta$. 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 $Y_\theta$ see the same field, they have identical trajec-
tories. As a result $X_\theta$ cannot be simultaneously steered from
$(0, 0, 1)$ to $(1, 0, 0)$. Lack of ensemble controllability
also be understood by looking at Lie brackets of the
generators. Equation (3) can be written as

$$\dot{X}_\theta = \{A(t) \cos(\phi(t)) B_1 + A(t) \sin(\phi(t)) \} X_\theta,$$

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 $B_3's$ 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 $\theta$.

**Example 4:** 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 $\omega$.

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

$$\exp(\pi \Omega_x) \exp(\omega \Omega_z dt) \exp(-\pi \Omega_x) = \exp(-\omega \Omega_z dt). \quad (4)$$

Now as before a maneuver

$$\exp(-\omega \Omega_z \sqrt{dt}) \exp(-\pi \Omega_x \sqrt{dt}) \exp(\omega \Omega_z \sqrt{dt})$$

produces the bracket direction $[\omega \Omega_z, \Omega_x] = \omega \Omega_y$ to lead-
ning order. Similarly $[\omega \Omega_z, [\omega \Omega_z, \Omega_x]] = -\omega^2 \Omega_x$. Hence,
we can generate higher brackets with even and odd pow-
ers of $\omega$. To see that the system is ensemble controllable
consider the Lie bracket relation $ad_{[\omega \Omega_z, \Omega_x]} = (-1)^n \omega^{2n} \Omega_x$ and $ad_{[\omega \Omega_z, \Omega_x]} = (-1)^{n+1} \omega^{2n+1} \Omega_x$.

We can synthesize an evolution $\exp(\sum_k c_k \omega^k \Omega_x)$ and sim-
ilarly the evolution $\exp(\sum_k d_k \omega^k \Omega_y)$. The coefficients
$c_k$ and $d_k$ can be chosen to approximate Euler angles
$(\alpha(\omega), \beta(\omega), \gamma(\omega))$ and we therefore as in Theorem 1, have
ensemble controllability.

**Remark** Note if we have only one quadrature of the
control field i.e.,

$$\dot{X} = (\omega \Omega_z + u(t) \Omega_x) X,$$

then we can only synthesize the generator $\Omega_y$ with odd
powers of $\omega$, with $\omega \in [-B, B]$. Therefore an evolu-
tion of the form $\exp(f(\omega) \Omega_y)$ cannot be approximated if $f$
 is an even function.

**Example 5:** Dispersion in Coupling Strengths

Consider two coupled qubits with Ising type interactions
with dispersion in coupling strengths $J$. The interaction
Hamiltonian $H_c = J \sigma_1 \sigma_2$, with $J \in [J_1 - \delta, J_1 + \delta]$, $
\delta > 0$. Although not necessary, for simplicity of exposition,
we assume that we can produce local unitary trans-
formation on the qubits much faster than the evolution of
couplings. We now show that it is possible to com-
penate for dispersion in $J$ and generate any quantum logic
with high fidelity.

By local transformations we can synthesize the effective
Hamiltonian

$$J \sigma_1 \sigma_2 = \exp(i(\pi \Omega_x / 2) (J \sigma_1 \sigma_2)) \exp(-i(\pi \Omega_x / 2)).$$

Now using $B_1 = -i2\sigma_1 \sigma_2$ and $B_2 = -i2\sigma_1 \sigma_2$ as gen-
erators we get $[J B_1, B_2] = -iJ^3 B_2$. Now using a con-
struction similar to one in example 1, we can syn-
thesize the evolution $\exp(\sum_k c_k J^{2k+1} \sigma_1 \sigma_2)$, where the
coefficients $c_k$ are chosen such that $\sum_k c_k J^{2k+1} = J_0$ over
the range of dispersion of $J$. Hence we have compensate
dispens in $J$. We also have ensemble controllability
with respect to the parameter $J$. Let

$$A(\sigma_1 \sigma_2) = \exp(-i(a(\sigma_1 \sigma_2) + b(\sigma_1 \sigma_2) + c(\sigma_1 \sigma_2)).$$

We can write an arbitrary two qubit gate with the depend-
cy on $J$ as

$$U_2(J) \otimes U_1(J) A(\sigma_1 \sigma_2) U_2(J) \otimes V_1(J),$$

where $U_1$ and $U_2$ are local unitaries on qubits 1 and 2 respec-
tively. We can synthesize them with a explicit depend-
cence on $J$ as follows. Using the commuta-
tions of the relations of the type $[-iJ^2, \sigma_1 \sigma_2, -iJ^2, \sigma_1 \sigma_2] = \sigma_1 \sigma_2$, $J^2 \sigma_2$, $-i(J^2)^k \sigma_1 \sigma_2$, $-i(J^2)^k \sigma_1 \sigma_2$, $-i(J^2)^k \sigma_1 \sigma_2$ ($k = 0, 1, 2, \ldots$ )
and use these to synthesize $U_1(J), V_1(J), U_2(J), V_2(J)$.

**Remark** Using similar ideas as above, it is possible to com-
nensate for more general coupling tensor. Consider the
coupling tensor

$$a \sigma_1 \sigma_2 + b \sigma_1 \sigma_2 + c \sigma_1 \sigma_2,$$

with dispersion in $\alpha, \beta, \gamma$. Now observe for $U = \exp(-i\pi \sigma_x)$, and $A = \exp(-i(a \sigma_1 \sigma_2 + b \sigma_1 \sigma_2 + c \sigma_1 \sigma_2))$.

$$U A U^\dagger A = \exp(-i\gamma 2 \sigma_1 \sigma_2).$$

So we only need to take care of the dispersion in $\gamma$ and
the construction is similar to the one before.
III. ENSEMBLE CONTROLLABILITY OF THE BLOCH EQUATIONS WITH BOUNDED CONTROLS

We consider again the system (11) but now with bounded controls, so that we cannot produce rotations of the type \( \exp(-i\Omega_x \pi) \) in arbitrarily small time as in equation (4). Nonetheless the system is still ensemble controllable as shown below. Our construction initially follows the well known algorithm of Shinnar-Roux [13, 14]. 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 \( R \in SO(3) \). We work with \( SU(2) \) representation of these rotations. Recall a rotation by angle \( \phi \) around the unit vector \((n_x, n_y, n_z)\) has a \( SU(2) \) representation of the form

\[ U = \begin{bmatrix} \alpha & -\beta^* \\ \beta & \alpha^* \end{bmatrix}, \quad (5) \]

where \( \alpha \) and \( \beta \) are the Cayley-Klein parameters satisfying

\[ \alpha = \cos \frac{\phi}{2} - i n_z \sin \frac{\phi}{2}, \]
\[ \beta = -i(n_x + i n_y) \sin \frac{\phi}{2}, \]
\[ \alpha \alpha^* + \beta \beta^* = 1. \quad (8) \]

The Bloch equation then takes the form

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

The rotation \( U \) is simply represented by its first column (also termed spinor representation) \( \psi = \begin{bmatrix} \alpha \\ \beta \end{bmatrix} \). We first consider piecewise-constant controls \( u(t) \) and \( v(t) \). The net rotation under these controls can be represented as successive rotations

\[ U = U_n U_{n-1} \ldots U_1 U_0, \]

where \( U_j = \begin{bmatrix} a_j & -b_j^* \\ b_j & a_j^* \end{bmatrix} \) and \( a_j, b_j \) are the Cayley-Klein parameters for the \( j \)th interval. Defining the multiplication of the matrices \( U_j \) up to \( k \) by

\[ \begin{bmatrix} \alpha_k & -\beta_k^* \\ \beta_k & \alpha_k^* \end{bmatrix} = \begin{bmatrix} a_k & -b_k^* \\ b_k & a_k^* \end{bmatrix} \ldots \begin{bmatrix} a_0 & -b_0^* \\ b_0 & a_0^* \end{bmatrix}, \]

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

\[ \begin{bmatrix} \alpha_k \\ \beta_k \end{bmatrix} = \begin{bmatrix} a_k & -b_k^* \\ b_k & a_k^* \end{bmatrix} \begin{bmatrix} \alpha_{k-1} \\ \beta_{k-1} \end{bmatrix}, \quad (9) \]

with the initial condition \( \begin{bmatrix} \alpha_0 \\ \beta_0 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \). The duration \( \Delta t \), 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

\[ e^{(\omega \Omega_z + u \Omega_y - v \Omega_z) \Delta t} \approx e^{(u \Omega_y - v \Omega_z) \Delta t} e^{\omega \Omega_z \Delta t}. \]

Under this assumption, we can write the rotation \( U_k \) as a rotation around \( z \)-axis by an angle \( \phi_k \) followed by a rotation about the applied control fields by an angle \( \phi_k \) in \( SU(2) \) representation

\[ U_k = \begin{bmatrix} C_k & -S_k^* \\ S_k & C_k \end{bmatrix} \begin{bmatrix} z^{1/2} & 0 \\ 0 & z^{-1/2} \end{bmatrix}, \quad (10) \]

where

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

Plugging (10) into (9), we get the recursion relation of the spinor

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

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

\[ \begin{bmatrix} P_k \\ Q_k \end{bmatrix} = \begin{bmatrix} C_k & -S_k^* \\ S_k & C_k \end{bmatrix} \begin{bmatrix} P_{k-1} \\ Q_{k-1} \end{bmatrix}, \quad (12) \]

with the initial condition

\[ \begin{bmatrix} P_0 \\ Q_0 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}. \quad (13) \]

Having the recursion (12) and the initial condition (13), the spinor at the \( n \)th step can be represented as the \( (n-1) \)-order polynomials in \( z \) (the parameter \( z \) encodes the dispersion parameter \( \omega \)).

\[ P_n(z) = \sum_{k=0}^{n-1} p_k z^{-k}, \quad (14) \]
\[ Q_n(z) = \sum_{k=0}^{n-1} q_k z^{-k}. \quad (15) \]

Note that

\[ |P_n(z)|^2 + |Q_n(z)|^2 = 1, \quad (16) \]

which follows from (3). The representation of rotation produced by the controls \( u(t) \) and \( v(t) \) has now been reduced from a product of \( n \) matrices in \( SU(2) \) to two \( (n-1) \)-order polynomials. The desired final states of an
ensemble of systems in (11), described by Cayley-Klein parameters, are two functions of \( z \), and hence of \( \omega \). 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 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 by multiplying both sides of (12) by the inverse of the rotation matrix we get

\[
\begin{bmatrix}
P_{k-1} \\
Q_{k-1}
\end{bmatrix} = \begin{bmatrix}
C_k P_k + S_k^* Q_k \\
- S_k P_k + C_k Q_k
\end{bmatrix},
\]

and the constraint of (10) is still preserved. 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 \( Q_{k-1}(z) \). This is the well known Shinnar Roux [13, 14] algorithm. Because \( P_{k-1}(z) \) and \( Q_{k-1}(z) \) are lower order polynomials, the leading term in \( P_{k-1} \) and the low-order term in \( Q_{k-1}(z) \) must drop out

\[
P_{k-1} P_{k,0} + Q_{k-1} Q_{k,0} = 0, \tag{18}
\]

\[
- S_k P_{k,0} + C_k Q_{k,0} = 0, \tag{19}
\]

where \( P_{k,m} \) denotes the coefficient of \( z^{-m} \) term in \( P_k(z) \). Observe that these two equations are equivalent as may be seen by expanding (10) as a polynomial,

\[
P(z) = \sum_{m=0}^{n-1} \sum_{i=0}^{m} \left[ P_i P_{m-i} + Q_i Q_{m-i} \right] z^{-m} = 1,
\]

and noting that all but the constant term are zero. The coefficient of \( z^{-(k-1)} \) in \( P(z) \) gives

\[
\frac{P_{k,k-1} P_{k,0} + Q_{k,k-1} Q_{k,0}}{P_{k,0}} = 0.
\]

With this relation either equation (18) or (19) may be derived from the other. Choosing (19) and combining it with (12), we get

\[
\frac{Q_{k,0}}{P_{k,0}} = -ie^{i\phi_k} \sin \frac{\phi_k}{2}, \tag{20}
\]

This gives the rotation angle

\[
\phi_k = 2 \tan^{-1} \left| \frac{Q_{k,0}}{P_{k,0}} \right|. \tag{21}
\]

Combining (20) and (21), we obtain the phase of the controls

\[
\theta_k = \angle \left( \frac{i Q_{k,0}}{P_{k,0}} \right).
\]

The controls \( u_k \) and \( v_k \) are then

\[
u_k = \frac{\phi_k}{\Delta t} \sin \theta_k, \tag{22}
\]

\[
v_k = \frac{\phi_k}{\Delta t} \cos \theta_k.
\]

These expressions for controls coupled with the inverse recursion in (17) 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 \( Q_n(z) = -i \sin \frac{\phi}{2} \) and \( P_n(z) = \cos \frac{\phi}{2} \), we obtain a broadband rotation around \( x \) axis by angle \( \phi \) and similarly by choosing \( Q_n(z) = \sin \frac{\phi}{2} \) and \( P_n(z) = \cos \frac{\phi}{2} \), we obtain an approximation to a broadband rotation around \( y \) axis by angle \( \phi \).

If the amplitude of the controls is bounded, we can choose \( \phi \) small enough so that it can be achieved by small flip angles \( \phi_k \) in equation (22). Now we can concatenate these rotations to achieve a rotation with a bigger angle and thereby maintain the bounds on the control.

Now we consider the case when there is also rf-inhomogeneity. If we produce a small flip angles \( \phi \) compensating for dispersion in \( \omega \), then dispersion \( \epsilon \) in the strength of the control \( u \) and \( v \), results in \( Q_n(z,\epsilon) \approx -ie^{i\phi_k} \frac{\phi_k}{2} \epsilon \) and the ensemble executes an effective rotation \( \exp(-ie^{i\phi_k} \sigma_z + i \sin(\theta_k) \sigma_y) \). Now using methods of example one, we can concatenate many such rotations to compensate for \( \epsilon \). We now show ensemble controllability with respect to both dispersion in the natural frequency \( \omega \) and strength of the rf-field.

We again write the final rotation \( U \in SU(2) \) as

\[
U = U_n U_{n-1} \ldots U_1 U_0,
\]

where

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

Note that the flip angle has a dependence on the parameter \( \epsilon \). We can now choose a desired \( Q_n(z,\epsilon) = \sum_{k=0}^{n-1} q_k(z,\epsilon) z^{-k} \) and \( P_n(z,\epsilon) = \sum_{k=0}^{n-1} p_k(z,\epsilon) z^{-k} \) and find the flip angles \( (\theta_k(\epsilon),\phi_k(\epsilon)) \) that creates these polynomials. Now we can use the results of Example 1 to find pulse sequences that will synthesize \( (\theta(\epsilon),\phi(\epsilon)) \). This then establishes the ensemble controllability with respect to both \( \omega \) and \( \epsilon \). Such constructions can also be used to generate pattern pulses that selectively excite the Bloch equations with parameters lying in a given subset of \( \omega - \epsilon \) space \( S \).

We now investigate the subject of ensemble control from a general control theory perspective.

\section*{IV. ENSEMBLE CONTROLLABILITY}

Consider a family of control systems

\[
\frac{dx_s}{dt} = f_s(x_s, u, t), \tag{23}
\]

indexed by the parameter vector \( s \) taking values in some compact set \( \Omega \subset \mathbb{R}^d \). The same control \( u(t) \in \mathbb{R}^m \) is
being used to simultaneously steer this family of control systems. For such systems, we define the notion of ensemble controllability as following.

**Definition 1** The family of systems in \( \mathcal{L} \) is called *ensemble controllable*, if there exists a control law \( u(t) \) such that starting from any initial state \( x_s(0) \), the system can be steered to within a ball of radius \( \epsilon \) around the target state \( g_s \), i.e. \( \| x_s(T) - g_s \| < \epsilon \). Here \( x_s(0) \) and \( x_s(T) \) are interpreted as functions of the variable \( s \) at time 0 and \( T \) and \( \| \cdot \| \) denotes a desired norm on function space. In this paper we take \( \| \cdot \| \) to denote \( L_2 \) norm. The final time \( T \) may depend on \( \epsilon \).

**Definition 2** An ensemble of systems is called *point ensemble controllable* if both the initial state \( x_s(0) \) and the target state \( g_s \) are constant functions and the ensemble of systems can be steered between the initial and final states as defined above.

The key problem of interest in ensemble controllability is to characterize the properties of the ensemble such that if each system of the ensemble is controllable, the whole family is ensemble controllable. We begin with considering linear systems \( \dot{x} = Ax + Bu \), where \( B \) is a \( n \times m \) matrix and \( u \in \mathbb{R}^m \).

**Theorem 1 (A negative result):** An ensemble of linear control systems is not ensemble controllable if there is a variation in the control matrix \( B \).

**Proof:** Consider the family of systems

\[
\frac{dx_s}{dt} = (Ax_s + B_s u).
\]

By variation of constant formula

\[
x_s(T) = \exp(AT)x_s(0) + \exp(AT) \int_0^T \exp(-A\tau)B_s u(\tau)d\tau.
\]

Since \( x_s(T) \) is linear in control, variation in \( B \) in general makes the system ensemble uncontrollable.

**Remark** Observe \( B_s u = \sum_{k=1}^m u_k b_k \) where \( b_k \) are the columns of \( B \). We can think of \( b_k \) as constant vector fields that generate translations. Since all \( b_k \) commute, their Lie brackets do not generate terms carrying higher powers of the dispersion parameters.

**Theorem** Consider an ensemble \((A, b)_s\), of linear single input controllable systems

\[
\dot{x} = A_s x + ub_s.
\]

The system is ensemble controllable only if distinct \( A_s \) have distinct eigenvalues and \( A_s \) is full rank over the ensemble.

**Proof:** Since each of the systems is controllable, there exists a similarity transformation \( T_s \) such that

\[
A_s = T_s^{-1} \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 & 1 \\ -a_0^s & -a_1^s & \cdots & -a_{n-2}^s & a_{n-1}^s \end{bmatrix} T_s
\]

and

\[
b = T_s^{-1} \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}
\]

where \( a_i^s \) are the coefficients of the characteristic polynomial of \( A_s \) and show dispersion over the ensemble. First observation is that for the ensemble to be controllable, we must have \( T_s \) to be a explicit function of \((a_0^s, a_1^s, a_2^s, \ldots, a_{n-1}^s)\). Suppose two distinct \( T_1 \) and \( T_2 \) correspond to the same \((a_0, a_1, a_2, \ldots, a_{n-1})\), then starting from \( x = 0 \), for equation (25), the final points \( x_1 \) and \( x_2 \) for the two systems at any time \( t \) are related by \( x_1(t) = T_1 T_2^{-1} x_2(t) \). Hence there exists no control that steers the two systems to the same point starting from 0. Therefore \( T_s \) should be a function of \((a_0^s, a_1^s, a_2^s, \ldots, a_{n-1}^s)\), i.e. no two distinct \( A \) have the same characteristic polynomial. We now show the necessity of \( A \) to be full rank. Observe if \( A \) is not full rank, i.e., \( a_0^s = 0 \), then \( A^k b \) for \( k > 0 \) always lies in the subspace \( H = span\{A^ib\}_{i=1}^{n-1} \). Therefore the ensemble starting from \( x = 0 \), cannot be driven to a final state \( f(a_1^s, a_2^s, \ldots, a_{n-1}^s) b \), where \( f \) is an arbitrary smooth scalar function of \((a_1^s, a_2^s, \ldots, a_{n-1}^s)\).

**Remark** As mentioned before the key idea in designing compensating pulse sequence is to synthesize higher order Lie brackets that raise the dispersion parameters to higher powers. As a result nilpotent control systems are not ensemble controllable as we cannot generate a desired higher power of the dispersion parameter. Consider the control system

\[
\dot{x} = \sum_i u_i(t) e_i g_i(x).
\]

If the Lie algebra generated by \( g_i \) is nilpotent, the system is not ensemble controllable.

**Example** Consider the well studied nonholonomic integrator

\[
\frac{d}{dt} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = u_1 \epsilon \begin{bmatrix} 1 \\ 0 \\ -x_2 \end{bmatrix} + u_2 \epsilon \begin{bmatrix} 0 \\ 1 \\ x_1 \end{bmatrix}.
\]

The system is not ensemble controllable with respect to the parameter \( \epsilon \). The control vector fields \( g_1 = \frac{\partial}{\partial x_1} - x_2 \frac{\partial}{\partial x_2} \) and \( g_2 = \frac{\partial}{\partial x_2} - x_1 \frac{\partial}{\partial x_3} \) generate a nilpotent algebra
the Heisenberg algebra. Observe that $[\epsilon g_1, \epsilon g_2] = 2\epsilon^2 \partial_3$, which commutes with everything else.

**Remark** Let $G$ be a semi-simple Lie group and let $X \in G$. Consider the control system

$$\dot{X} = \left( \sum_i u_i \epsilon_i B_i \right) X,$$

such that $\epsilon_i$ have dispersion in the range $[1-\delta_i, 1+\delta_i]$, for $\delta_i > 0$. If Lie algebra generated by $\{B_i\}$ spans the tangent space of $G$, then the system is ensemble controllable. The construction is similar in spirit to example 2.

In this paper, we have tried to motivate the study of problems involving control of ensembles of dynamical systems with dispersion in the parameters. Such problems arise naturally in areas of coherent spectroscopy, quantum information processing and control of quantum systems in general. We have tried to make explicit the role of noncommutativity as a key aspect of the dynamics that makes design of a compensating control signal possible. We note again that the constructions given in this paper do not provide the most efficient schemes for compensation, yet they illustrate the main ideas of the paper in a transparent way. The subject of ensemble control appears to be very rich and we anticipate that many interesting results of both theoretical and practical importance will arise from a systematic study in this field.

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