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Complete controllability of finite-level quantum systems

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Abstract

Complete controllability is a fundamental issue in the field of control of quantum systems, not least because of its implications for dynamical realizability of the kinematical bounds on the optimization of observables. In this paper we investigate the question of complete controllability for finite-level quantum systems subject to a single control field, for which the interaction is of dipole form. Sufficient criteria for complete controllability of a wide range of finite-level quantum systems are established and the question of limits of complete controllability is addressed. Finally, the results are applied to give a classification of complete controllability for four-level systems.

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1. Introduction

Recent advances in laser technology have opened up new possibilities for laser control of quantum phenomena such as control of molecular quantum states, chemical reaction dynamics or quantum computers. The limited success of initially advocated control schemes based largely on physical intuition in both theory and experiment has prompted researchers in recent years to study these systems using control theory [1].

In [2] it was shown that the kinematical constraint of unitary evolution for non-dissipative quantum systems gives rise to universal, kinematical bounds on the optimization of observables. It has also been demonstrated that the theoretically and practically important question of the dynamical realizability of these universal bounds depends on the complete controllability of the system [3]. Although the issue of complete controllability of quantum systems has been investigated before [4, 7], many open questions remain.

In this paper we study the question of complete controllability of finite-level quantum systems driven by a single control, for which the interaction with the control field is determined by the dipole approximation. For this kind of system the total Hamiltonian is of the form

$$H = H_0 + f(t)H_1 \tag{1}$$

where H_0 is the internal system Hamiltonian and H_1 is the interaction Hamiltonian. For a finite-level quantum system there always exists a complete orthonormal set of energy eigenstates $|n\rangle$ such that $H_0|n\rangle = E_n|n\rangle$ and thus we have

$$H_0 = \sum_{n=1}^{N} E_n|n\rangle\langle n| = \sum_{n=1}^{N} E_n e_{nn} \tag{2}$$

where $e_{mn} \equiv |m\rangle\langle n|$ is an $N \times N$ matrix with elements $(e_{mn})_{kl} = \delta_{mk}\delta_{nl}$ and E_n are the energy levels of the system. The E_n are real and hence H_0 is Hermitian. The system is non-degenerate provided that $E_n = E_m$ if and only if $m = n$. The energy levels can be ordered in a non-increasing sequence, i.e., $E_1 \leqslant E_2 \leqslant \ldots \leqslant E_N$. Hence, the energy level spacing is

$$\mu_n \equiv E_{n+1} - E_n \geqslant 0 \qquad n = 1, \ldots, N-1. \tag{3}$$

If $\mu_n = \mu$ for $1 \leqslant n \leqslant N-1$ then we say the energy levels are equally spaced.

Expanding the interaction Hamiltonian H_1 with respect to this complete set of orthonormal energy eigenstates $|n\rangle$ leads to

$$H_1 = \sum_{m,n=1}^{N} d_{m,n}|m\rangle\langle n|$$

where $d_{m,n}$ are the transition dipole moments, which satisfy $d_{m,n} = d^*_{n,m}$, where $d^*_{n,m}$ is the complex conjugate of $d_{n,m}$. Thus, H_1 is Hermitian. In the dipole approximation it is generally assumed that only the terms $d_{n-1,n}$ and $d_{n,n-1}$ corresponding to transitions between adjacent energy levels are relevant, i.e., $d_{m,n} = 0$ unless $m = n \pm 1$. Thus, letting $d_n = d_{n,n+1}$ for $1 \leqslant n \leqslant N-1$ we have

$$H_1 = \sum_{n=1}^{N-1} d_n(|n\rangle\langle n+1| + |n+1\rangle\langle n|) = \sum_{n=1}^{N-1} d_n(e_{n,n+1} + e_{n+1,n}). \tag{4}$$

If the any of the d_n for $1 \leqslant n \leqslant N-1$ vanish then the system is decomposable, i.e., its dynamics can be decomposed into independent subspace dynamics, and therefore not completely controllable [3]. Hence, we shall assume that

$$d_n \neq 0 \qquad 1 \leqslant n \leqslant N-1 \qquad d_0 = d_N = 0. \tag{5}$$

Note that we have introduced the non-physical $d_0 = d_N = 0$ for convenience.

2. Sufficient conditions for complete controllability

Definition 1. *A quantum system $H = H_0 + f(t)H_1$ is* completely controllable *if every unitary operator is dynamically accessible from the identity I in $U(N)$ via a path $\gamma(t) = U(t, t_0)$ that satisfies the equation of motion*

$$\mathrm{i}\hbar\frac{\partial}{\partial t}U(t, t_0) = (H_0 + f(t)H_1)U(t, t_0) \tag{6}$$

with initial condition $U(t_0, t_0) = I$.

In [4,5] it was shown that a necessary and sufficient condition for complete controllability of the system $H = H_0 + f(t)H_1$ is that the Lie algebra $\mathcal{L}$ generated by the skew-Hermitian matrices $\mathrm{i}H_0$ and $\mathrm{i}H_1$ is $u(N)$, i.e., the Lie algebra of skew-Hermitian $N \times N$ matrices. Note that we have $u(N) = su(N) \oplus u(1)$ where $su(N)$ is the Lie algebra of traceless skew-Hermitian matrices. A standard basis for $su(N)$ is [6]

$$\begin{aligned} x_{nn'} &\equiv e_{nn'} - e_{n'n} \\ y_{nn'} &\equiv \mathrm{i}(e_{nn'} + e_{n'n}) \\ h_n &\equiv \mathrm{i}(e_{nn} - e_{n+1,n+1}) \end{aligned} \tag{7}$$

where $1 \leqslant n \leqslant N-1$, $n < n' \leqslant N$ and $\mathrm{i} = \sqrt{-1}$. However, to show that $\mathcal{L}$ contains $su(N)$, it is sufficient to prove that $x_{n,n+1}, y_{n,n+1} \in \mathcal{L}$ for $1 \leqslant n \leqslant N-1$ since all other basis elements can be generated recursively from $x_{n,n+1}$ and $y_{n,n+1}$ for $k > 1$:

$$\begin{aligned} x_{n,n+k} &= [x_{n,n+k-1}, x_{n+k-1,n+k}] \\ y_{n,n+k} &= [y_{n,n+k-1}, x_{n+k-1,n+k}] \\ h_n &= [x_{n,n+1}, y_{n,n+1}]. \end{aligned}$$

If $\mathrm{Tr}(H_0) = 0$ then the Lie algebra $\mathcal{L}$ can be at most $su(N)$ since H_1 is traceless by definition. Note that it can be shown that $\mathcal{L} = su(N)$ is sufficient for controllability for many practical purposes [7]. On the other hand, if $su(N) \subset \mathcal{L}$ and $\mathrm{Tr}(H_0) \neq 0$ then $\mathrm{i}I$ can be obtained from the diagonal element $\mathrm{i}H_0 \in \mathcal{L}$ since we can write

$$\mathrm{i}H_0 = \left[N^{-1}\mathrm{Tr}(H_0)\right]\mathrm{i}I + H_0' \tag{8}$$

where the traceless matrix H_0' must be a real linear combination of h_n and hence in the Lie algebra $\mathcal{L}$. Thus, if $su(N) \subset \mathcal{L}$ and $\mathrm{Tr}(H_0) \neq 0$ then $\mathcal{L} = u(N)$.

For a system $H = H_0 + f(t)H_1$ with interaction Hamiltonian H_1 of the form (4), it turns out that it actually suffices to show that $x_{p,p+1}, y_{p,p+1} \in \mathcal{L}$ for some p and $d_{p-k} \neq \pm d_{p+k}$ for some k in order to conclude that $\mathcal{L}$ contains $su(N)$.

Lemma 1. *If $x_{12}, y_{12} \in \mathcal{L}$ then $x_{n,n+1}, y_{n,n+1} \in \mathcal{L}$ for $1 \leqslant n \leqslant N-1$. Similarly, if $x_{N-1,N}, y_{N-1,N} \in \mathcal{L}$ then $x_{n,n+1}, y_{n,n+1} \in \mathcal{L}$ for $1 \leqslant n \leqslant N-1$.*

Proof. Given $x_{12}, y_{12} \in \mathcal{L}$, let $V = \mathrm{i}H_1$ and

$$\begin{aligned} h_1 &\equiv 2^{-1}[x_{12}, y_{12}] = \mathrm{i}(e_{11} - e_{22}) \\ V^{(1)} &\equiv V - d_1 y_{12} = \sum_{n=2}^{N-1} d_n y_{n,n+1}. \end{aligned}$$

Since $d_n \neq 0$ for $1 \leqslant n \leqslant N-1$ we find that

$$d_2^{-1}[h_1, V^{(1)}] = x_{23} \in \mathcal{L} \qquad [x_{23}, h_1] = y_{23} \in \mathcal{L}.$$

By repeating this procedure $N-2$ times, we can show that $x_{n,n+1}, y_{n,n+1} \in \mathcal{L}$ for $1 \leqslant n \leqslant N-1$. Similarly, we can prove that given $x_{N-1,N}, y_{N-1,N} \in \mathcal{L}$ then all $x_{n,n+1}, y_{n,n+1} \in \mathcal{L}$ for $1 \leqslant n \leqslant N-1$. □

Lemma 2. *If there exists p with $2 \leqslant p \leqslant N-2$ such that $x_{p,p+1}, y_{p,p+1} \in \mathcal{L}$ and k such that $d_{p-k} \neq \pm d_{p+k}$ then $x_{n,n+1}, y_{n,n+1} \in \mathcal{L}$ for $1 \leqslant n \leqslant N-1$.*

Proof. Given $x_{p,p+1}, y_{p,p+1} \in \mathcal{L}$ with $2 \leqslant p \leqslant N-2$ then

$$h_p \equiv 2^{-1}[x_{p,p+1}, y_{p,p+1}] = \mathrm{i}(e_{pp} - e_{p+1,p+1}) \in \mathcal{L}.$$

Next let $V = \mathrm{i}H_1$ and evaluate

$$\begin{aligned} V_p^{(1)} &\equiv V - d_p y_{p,p+1} = \sum_{n \neq p} d_n y_{n,n+1} \\ X_p^{(1)} &\equiv d_{p-1}^{-1}[h_p, V_p^{(1)}] = x_{p-1,p} + \eta_p^{(1)} x_{p+1,p+2} \\ Y_p^{(1)} &\equiv [X_p^{(1)}, h_p] = y_{p-1,p} + \eta_p^{(1)} y_{p+1,p+2} \\ H_p^{(1)} &\equiv 2^{-1}[X_p^{(1)}, Y_p^{(1)}] = h_{p-1} + (\eta_p^{(1)})^2 h_{p+1} \\ X_p^{(1)'} &\equiv 2^{-1}[Y_p^{(1)}, H_p^{(1)}] = x_{p-1,p} + (\eta_p^{(1)})^3 x_{p+1,p+2} \\ Y_p^{(1)'} &\equiv 2^{-1}[H_p^{(1)}, X_p^{(1)}] = y_{p-1,p} + (\eta_p^{(1)})^3 y_{p+1,p+2} \end{aligned}$$

where $\eta_p^{(1)} = d_{p+1}/d_{p-1}$. Note that $\eta_p^{(1)}$ is defined and non-zero since by hypothesis $d_n \neq 0$ for $1 \leqslant n \leqslant N-1$. This leads to

$$(\eta_p^{(1)})^2 X_p^{(1)} - X_p^{(1)'} = [(\eta_p^{(1)})^2 - 1] x_{p-1,p} \in \mathcal{L}$$
$$(\eta_p^{(1)})^2 Y_p^{(1)} - Y_p^{(1)'} = [(\eta_p^{(1)})^2 - 1] y_{p-1,p} \in \mathcal{L}.$$

At this point we have to distinguish two cases.

Case 1. If $\eta_p^{(1)} \neq \pm 1$, i.e., $d_{p-1} \neq \pm d_{p+1}$, then it is easy to see that $x_{p-1,p}, y_{p-1,p} \in \mathcal{L}$ and hence $h_{p-1} \equiv 2^{-1}[x_{p-1,p}, y_{p-1,p}] \in \mathcal{L}$ as well. Now we can proceed to show that $x_{p-2,p-1}, y_{p-2,p-1} \in \mathcal{L}$:

$$V_p^{(2)} \equiv V_p^{(1)} - d_{p-1} y_{p-1,p}$$
$$X_p^{(2)} \equiv d_{p-2}^{-1}[h_{p-1}, V_p^{(2)}] = x_{p-2,p-1} \in \mathcal{L}$$
$$Y_p^{(2)} \equiv [X_p^{(2)}, h_{p-1}] = y_{p-2,p-1} \in \mathcal{L}.$$

Repeating the last step $p-2$ times shows that $X_p^{(p-1)} = x_{12} \in \mathcal{L}$ and $Y_p^{(p-1)} = y_{12} \in \mathcal{L}$ and hence $x_{n,n+1}, y_{n,n+1} \in \mathcal{L}$ for $1 \leqslant n \leqslant N-1$ by lemma 1.

Case 2. If $\eta_p^{(1)} = \pm 1$, i.e., $d_{p-1} = \pm d_{p+1}$, then we only have $X_p^{(1)'} = x_{p-1,p} \pm x_{p+1,p+2} \in \mathcal{L}$ and $Y_p^{(1)'} = y_{p-1,p} \pm y_{p+1,p+2} \in \mathcal{L}$. However, we can now use a similar procedure as above to obtain

$$V_p^{(2)} \equiv V_p^{(1)} - d_{p-1} Y_p^{(1)'} = \sum_{n \neq p, p\pm 1} d_n y_{n,n+1}$$
$$H_p^{(2)} \equiv 2^{-1}[X_p^{(1)'}, Y_p^{(1)'}] = h_{p-1} + h_{p+1}$$
$$X_p^{(2)} \equiv d_{p-2}^{-1}[H_p^{(2)}, V_p^{(2)}] = x_{p-2,p-1} + \eta_p^{(2)} x_{p+2,p+3}$$
$$Y_p^{(2)} \equiv [X_p^{(2)}, H_p^{(2)}] = y_{p-2,p-1} + \eta_p^{(2)} y_{p+2,p+3}$$
$$H_p^{(2)'} \equiv 2^{-1}[X_p^{(2)}, Y_p^{(2)}] = h_{p-2} + (\eta_p^{(2)})^2 h_{p+2}$$
$$X_p^{(2)'} \equiv 2^{-1}[Y_p^{(2)}, H_p^{(2)'}] = x_{p-2,p-1} + (\eta_p^{(2)})^3 x_{p+2,p+3}$$
$$Y_p^{(2)'} \equiv 2^{-1}[H_p^{(2)'}, X_p^{(2)'}] = y_{p-2,p-1} + (\eta_p^{(2)})^3 y_{p+2,p+3},$$

where $\eta_p^{(2)} = d_{p+2}/d_{p-2}$. This leads to

$$(\eta_p^{(2)})^2 X_p^{(2)} - X_p^{(2)'} = [(\eta_p^{(2)})^2 - 1] x_{p-2,p-1} \in \mathcal{L}$$
$$(\eta_p^{(2)})^2 Y_p^{(2)} - Y_p^{(2)'} = [(\eta_p^{(2)})^2 - 1] y_{p-2,p-1} \in \mathcal{L}.$$

Again, we have to consider two different cases.

Case 2a. If $\eta_p^{(2)} \neq \pm 1$, i.e., $d_{p-2} \neq \pm d_{p+2}$, then $x_{p-2,p-1}, y_{p-2,p-1} \in \mathcal{L}$ as well as $h_{p-2} \equiv 2^{-1}[x_{p-2,p-1}, y_{p-2,p-1}] \in \mathcal{L}$ and we can proceed as in case 1 to show that $x_{p-3,p-2}, y_{p-3,p-2} \in \mathcal{L}$:

$$V_p^{(3)} \equiv V_p^{(2)} - d_{p-2} y_{p-2,p-1},$$
$$X_p^{(3)} \equiv d_{p-3}^{-1}[h_{p-2}, V_p^{(3)}] = x_{p-3,p-2} \in \mathcal{L}$$
$$Y_p^{(3)} \equiv [X_p^{(3)}, h_{p-2}] = y_{p-3,p-2} \in \mathcal{L}.$$

Repeating the last step $p-3$ times shows that $X_p^{(p-1)} = x_{12} \in \mathcal{L}$ and $Y_p^{(p-1)} = y_{12} \in \mathcal{L}$ and hence $x_{n,n+1}, y_{n,n+1} \in \mathcal{L}$ for $1 \leqslant n \leqslant N-1$ by lemma 1.

Case 2b. If $\eta_p^{(2)} = \pm 1$, i.e., $d_{p-2} = \pm d_{p+2}$, then we have only $X_p^{(2)} = x_{p-2,p-1} \pm x_{p+2,p+3} \in \mathcal{L}$ and $Y_p^{(2)} = y_{p-2,p-1} \pm y_{p+2,p+3} \in \mathcal{L}$ but we can proceed as in case 2 to obtain

$$X_p^{(3)\prime} = x_{p-3,p-2} + (\eta_p^{(3)})^3 x_{p+3,p+4} \in \mathcal{L}$$
$$Y_p^{(3)\prime} = y_{p-3,p-2} + (\eta_p^{(3)})^3 y_{p+3,p+4} \in \mathcal{L}$$

where $\eta_p^{(3)} = d_{p+3}/d_{p-3}$. Again, we must distinguish the cases $\eta_p^{(3)} \neq \pm 1$ and $\eta_p^{(3)} = \pm 1$ and so forth.

Using this procedure, we can always show that $x_{p-k,p-k+1}, y_{p-k,p-k+1} \in \mathcal{L}$ since by hypothesis $d_{p-k} \neq \pm d_{p+k}$. We can then proceed as in case 1 to show that $x_{12}, y_{12} \in \mathcal{L}$, from which it follows that all $x_{n,n+1}, y_{n+1,n} \in \mathcal{L}$ by lemma 1. □

3. Completely controllable quantum systems

3.1. Anharmonic systems

The results of the previous section can be applied to establish complete controllability for many quantum systems.

Theorem 1. *The dynamical Lie algebra for a quantum system $H = H_0 + f(t)H_1$ with H_0 and H_1 as in (2) and (4) is at least $su(N)$ if either*

(i) $\mu_1 \neq 0$ and $\mu_n \neq \mu_1$ for $2 \leqslant n \leqslant N-1$, or
(ii) $\mu_{N-1} \neq 0$ and $\mu_n \neq \mu_{N-1}$ for $1 \leqslant n \leqslant N-2$.

If in addition $\mathrm{Tr}(H_0) \neq 0$ then the dynamical Lie algebra is $u(N)$, i.e., the system is completely controllable.

Proof. Suppose $\mu_1 \neq 0$ and $\mu_n \neq \mu_1$ for $2 \leqslant n \leqslant N-1$. Let $V = \mathrm{i}H_1$ and evaluate

$$V' \equiv [\mathrm{i}H_0, V] = \sum_{n=1}^{N-1} \mu_n d_n x_{n,n+1}$$

$$V'' \equiv [V', \mathrm{i}H_0] = \sum_{n=1}^{N-1} \mu_n^2 d_n y_{n,n+1}$$

$$V^{(1)} \equiv V'' - \mu_{N-1}^2 V = \sum_{n=1}^{N-2} (\mu_n^2 - \mu_{N-1}^2) d_n y_{n,n+1}$$

$$V^{(2)} \equiv [[\mathrm{i}H_0, V^{(1)}], \mathrm{i}H_0] - \mu_{N-2}^2 V^{(1)} = \sum_{n=1}^{N-3} (\mu_n^2 - \mu_{N-2}^2)(\mu_n^2 - \mu_{N-1}^2) d_n y_{n,n+1}$$

$$\vdots$$

$$V^{(k)} \equiv [[\mathrm{i}H_0, V^{(k-1)}], \mathrm{i}H_0] - \mu_{N-2}^2 V^{(k-1)} = \sum_{n=1}^{N-1-k} \left[\prod_{k=n+1}^{N-1} d_n (\mu_n^2 - \mu_k^2) \right] y_{n,n+1}$$

$$\vdots$$

$$V^{(N-2)} \equiv d_1 \left[\prod_{k=2}^{N-1} (\mu_1^2 - \mu_k^2) \right] y_{12} \in \mathcal{L}.$$

Since by hypothesis $d_1 \neq 0$, $\mu_1 \neq 0$ and $\mu_n \neq \mu_1$ for $2 \leqslant n \leqslant N-1$ we have $y_{12} \in \mathcal{L}$ and hence $\mu_1^{-1}[\mathrm{i}H_0, y_{12}] = x_{12} \in \mathcal{L}$. Hence, $su(N) \subset \mathcal{L}$ by lemma 1 and if $\mathrm{Tr}(H_0) \neq 0$ then $\mathcal{L} = u(N)$. The proof for the case $\mu_n \neq \mu_{N-1}$ for $1 \leqslant n \leqslant N-2$ is analogous. □

This theorem, first proved in [7], is very important in that it guarantees the complete controllability of physically important systems such as simple atomic systems or Morse oscillators, which are often used to model molecular bonds.

Example 1. The energy level spacing for a Morse oscillator is of the form $\mu_n \propto 1 - Bn$ where B is a small positive real number and we can assume $\mathrm{Tr}(H_0) \neq 0$. Therefore, $\mu_n \neq \mu_1$ for $n > 1$ and thus any N-level Morse oscillator system is completely controllable.

Theorem 1 also applies to degenerate or more complicated systems.

Example 2. Consider a system with energy levels E_1 and $E_n = E_2 \neq E_1$ for $2 \leqslant n \leqslant N$ with arbitrary non-zero transition dipole moments d_n. In this case we have $\mu_1 = E_2 - E_1 \neq 0$ but $\mu_n = 0$ for $2 \leqslant n \leqslant N-1$. Thus, surprisingly, this highly degenerate system is completely controllable by theorem 1 provided that $\mathrm{Tr}(H_0) \neq 0$.

Example 3. The energy levels of the bound states of a one-electron atom of atomic number Z are $E_n = (-13.9\ \mathrm{eV})Z^2/n^2$. Therefore, $\mathrm{Tr}(H_0) \neq 0$ and the energy level spacing is

$$\mu_n \propto n^{-2} - (n+1)^{-2} = \frac{(2n+1)}{n^2(n+1)^2}.$$

Note that the multiplicity of energy level E_n is $2n^2$ including angular momentum and spin degeneracy, i.e., the energy levels are degenerate. Nevertheless, we can apply theorem 1 to conclude that any non-decoupled N-level subsystem of this model consisting of at least two different energy levels is completely controllable if the interaction with the control field is of dipole form (4).

Example 4. The energy levels E_n for a particle in a 1D box are Cn^2, where C is a positive constant. Hence, $\mathrm{Tr}(H_0) \neq 0$ and $\mu_n \neq \mu_1$ for $n > 1$, i.e., any non-decoupled N-level subsystem of this model is completely controllable according to theorem 1 if the interaction with the control field is of dipole form (4).

Example 5. Consider a $(N = 2\ell+1)$-level system with $\mathrm{Tr}(H_0) \neq 0$ and energy level spacings $\mu_{2k} = \mu_2$ for $1 \leqslant k \leqslant \ell$ but $\mu_1 \neq \mu_n$ for $n > 1$. This system is also completely controllable (independent of the d_n) according to theorem 1. Similarly, if we had $\mu_{2k-1} = \mu_1$ for $1 \leqslant k \leqslant \ell$ but $\mu_{2\ell} \neq \mu_n$ for $n < 2\ell$ then the system would be completely controllable according to theorem 1 as well.

The last example is interesting for the following reason. Suppose we considered instead a composite system of ℓ coupled identical two-level systems with simple interactions, i.e., an $(N = 2\ell)$-level system with energy level spacings $\mu_{2k+1} = \mu_1$ for $1 < k < \ell$ but, for example, $\mu_2 \neq \mu_n$ for $n \neq 2$. In this case we have $\mu_1 = \mu_{2\ell-1}$, i.e., theorem 1 does not apply although considering the last example one would expect this system to be controllable as well. This suggests that theorem 1 can be generalized.

Theorem 2. *The dynamical Lie algebra $\mathcal{L}$ of a quantum system $H = H_0 + f(t)H_1$ with H_0 and H_1 as in (2) and (4) is at least $su(N)$ if there exists $\mu_p \neq 0$ such that $\mu_n \neq \mu_p$ for $n \neq p$, and k such that $d_{p-k} \neq \pm d_{p+k}$. If in addition* $\mathrm{Tr}(H_0) \neq 0$ *then $\mathcal{L} = u(N)$, i.e., the system is completely controllable.*

Proof. Let $V = \mathrm{i}H_1$ and define

$$\begin{aligned} V^{(1)} &\equiv [[\mathrm{i}H_0, V], \mathrm{i}H_0] - \mu_{\sigma(1)}^2 V \\ V^{(2)} &\equiv [[\mathrm{i}H_0, V^{(1)}], \mathrm{i}H_0] - \mu_{\sigma(2)}^2 V^{(1)} \\ &\vdots \\ V^{(N-2)} &\equiv [[\mathrm{i}H_0, V^{(N-3)}], \mathrm{i}H_0] - \mu_{\sigma(N-3)}^2 V^{(N-3)} \end{aligned}$$

where σ is a permutation of the set $\{1, 2, \ldots, N-1\}$ such that $\sigma(N-1) = p$. Then

$$V^{(N-2)} = d_p \left[\prod_{n=1}^{N-2} (\mu_p^2 - \mu_{\sigma(n)}^2) \right] y_{p,p+1} \in \mathcal{L}.$$

and since by hypothesis $d_p \neq 0$, $\mu_p \neq 0$ and $\mu_n \neq \mu_p$ for $n \neq p$ we have $y_{p,p+1} \in \mathcal{L}$ and hence $\mu_p^{-1}[\mathrm{i}H_0, y_{p,p+1}] = x_{p,p+1} \in \mathcal{L}$. By hypothesis we have furthermore $d_{p+k} \neq \pm d_{p-k}$ for some k. Hence, $su(N) \subset \mathcal{L}$ by lemma 2 and if $\mathrm{Tr}(H_0) \neq 0$ then $\mathcal{L} = u(N)$, i.e., the system is completely controllable. □

Note that $d_0 = d_N = 0$ and $d_n \neq 0$ for $1 \leqslant n \leqslant N-1$ implies that the condition $d_{p+k} \neq \pm d_{p-k}$ is always satisfied for $k = \min\{p, N-p\}$ unless $p = N-p$ since if $k = p < N-p$ then $d_{p-k} = d_0 = 0$ and $d_{p+k} \neq 0$, and if $k = N-p < p$ then $d_{p+k} = d_N = 0$ and $d_{p-k} \neq 0$. Furthermore, $p = N-p$ is only possible if $p = N/2$ and hence N even. Thus, assuming $\mathrm{Tr}(H_0) \neq 0$, we have the following:

Corollary 1. *If N is odd and there exists $\mu_p \neq 0$ such that $\mu_n \neq \mu_p$ for $n \neq p$, then the system is completely controllable.*

Corollary 2. *If N is even and there exists $\mu_p \neq 0$ with $p \neq N/2$ such that $\mu_n \neq \mu_p$ for $n \neq p$, then the system is completely controllable.*

Applying corollary 2 to the $(N = 2\ell)$-level composite system with energy level spacings $\mu_{2k+1} = \mu_1$ for $1 < k < \ell$ but $\mu_2 \neq \mu_n$ for $n \neq 2$ considered above, we see that the system is always controllable for $N \neq 4$. If $N = 4$ then it is controllable if $d_1 \neq \pm d_3$. There are many other applications for the theorems and corollaries above.

Example 6. The system of two coupled ℓ-level harmonic oscillators with

$$E_n = \begin{cases} E_1 + (n-1)\mu & \text{for } 1 \leqslant n \leqslant \ell \\ E_1 + (n-1)\mu + \Delta & \text{for } \ell + 1 \leqslant n \leqslant 2\ell \end{cases} \tag{9}$$

is completely controllable if $d_{\ell-k} \neq \pm d_{\ell+k}$ for some k since $\mu_n = \mu$ for $n \neq \ell$ and $\mu_\ell = \mu + \Delta$. For instance, if

$$d_n = \begin{cases} \sqrt{n} & \text{for } 1 \leqslant n \leqslant \ell - 1 \\ d \neq 0 & \text{for } n = \ell \\ \sqrt{n-\ell} & \text{for } \ell + 1 \leqslant n \leqslant 2\ell - 1 \end{cases} \tag{10}$$

then the system is completely controllable by theorem 2 since, e.g., $d_{\ell-1} = \sqrt{\ell - 1} \neq \sqrt{1} = d_{\ell+1}$. However, if

$$d_n = \begin{cases} 1 & \text{for } 1 \leqslant n \leqslant \ell - 1 \\ d \neq 0 & \text{for } n = \ell \\ 1 & \text{for } \ell + 1 \leqslant n \leqslant 2\ell - 1 \end{cases} \tag{11}$$

then the system does not satisfy the criteria for complete controllability established in the previous theorems and one can verify that the system is indeed not completely controllable.

3.2. Harmonic oscillators

Theorem 2 and its corollaries establish complete controllability for many anharmonic, non-decomposable quantum systems. However, the conditions on the μ_n exclude systems with equally spaced energy levels, i.e., $\mu_n = \mu$ for $1 \leqslant n \leqslant N-1$, such as harmonic oscillators. For these systems we cannot apply the techniques used in the previous section to establish complete controllability since in this case $[[\mathrm{i}H_0, V], \mathrm{i}H_0] = \mu V$. To resolve this problem, we introduce a new set of parameters depending on the values of the transition dipole moments d_n

$$v_n = 2d_n^2 - d_{n-1}^2 - d_{n+1}^2 \qquad 1 \leqslant n \leqslant N-1 \tag{12}$$

which determine whether the system is completely controllable or not.

Theorem 3. *The dynamical Lie algebra $\mathcal{L}$ for a system $H = H_0 + f(t)H_1$ with equally spaced energy levels, i.e., $\mu_n = \mu \neq 0$ for $1 \leqslant n \leqslant N-1$ is at least $su(N)$ if there exists $v_p \neq 0$ such that $v_n \neq v_p$ for $n \neq p$ and $p \neq N/2$; if $p = N/2$ then $d_{p-k} \neq \pm d_{p+k}$ for some k is required as well. If in addition $\mathrm{Tr}(H_0) \neq 0$ then $\mathcal{L} = u(N)$.*

Proof. For convenience we define $Y^{(1)} \equiv \mathrm{i}H_1$. Then we have

$$X^{(1)} \equiv \mu^{-1}[\mathrm{i}H_0, Y^{(1)}] = \sum_{n=1}^{N-1} d_n x_{n,n+1}$$

$$Z \equiv 2^{-1}[X^{(1)}, Y^{(1)}] = \mathrm{i}\sum_{n=1}^{N}(d_n^2 - d_{n-1}^2)e_{nn}.$$

From $X^{(1)}$, $Y^{(1)}$ and $Z^{(1)}$, we have

$$Y^{(2)} \equiv [Z, X^{(1)}] - v_{\sigma(1)}Y^{(1)} = \sum_{n=2}^{N-1}(v_n - v_{\sigma(1)})d_n y_{n,n+1}$$

$$X^{(2)} \equiv [Y^{(1)}, Z] - v_{\sigma(1)}X^{(1)} = \sum_{n=2}^{N-1}(v_n - v_{\sigma(1)})d_n x_{n,n+1}$$

$$Y^{(3)} \equiv [Z, X^{(2)}] - v_{\sigma(2)}Y^{(2)} = \sum_{n=3}^{N-1}(v_n - v_{\sigma(1)})(v_n - v_{\sigma(2)})d_n y_{n,n+1}$$

$$X^{(3)} \equiv [Y^{(2)}, Z] - v_{\sigma(2)}X^{(2)} = \sum_{n=3}^{N-1}(v_n - v_{\sigma(1)})(v_n - v_{\sigma(2)})d_n x_{n,n+1}$$

$$\vdots$$

$$Y^{(N-1)} \equiv [Z, X^{(N-2)}] - v_{\sigma(N-2)}Y^{(N-2)} = d_p\left[\prod_{n=1}^{N-2}(v_p - v_{\sigma(n)})\right] y_{p,p+1} \in \mathcal{L}$$

$$X^{(N-1)} \equiv [Y^{(N-2)}, Z] - v_{\sigma(N-2)}X^{(N-2)} = d_p\left[\prod_{n=1}^{N-2}(v_p - v_{\sigma(n)})\right] x_{p,p+1} \in \mathcal{L}.$$

where σ is a permutation of the set $\{1, 2, \ldots, N-1\}$ such that $\sigma(N-1) = p$. By hypothesis we have $v_p \neq 0$ and $v_n \neq v_p$ for $n \neq p$. Hence, we can conclude $x_{p,p+1}, y_{p,p+1} \in \mathcal{L}$. If $p \neq N/2$ then the condition $d_{p-k} \neq \pm d_{p+k}$ is automatically satisfied for $k = \min\{p, N-p\}$; otherwise it is guaranteed by the hypothesis of the theorem. Therefore, $\mathcal{L}$ contains $su(N)$ by lemma 2 and if $\mathrm{Tr}(H_0) \neq 0$ then $\mathcal{L} = u(N)$. □

Example 7. The truncated N-level harmonic oscillator with $E_n \propto n + \frac{1}{2}$ and $d_n = \sqrt{n}$ is completely controllable since $v_n = 0$ for $1 \leqslant n \leqslant N-2$ but $v_{N-1} = N \neq 0$.

Example 8. A system with N equally spaced energy levels, $\mathrm{Tr}(H_0) \neq 0$, and $d_n = 1$ for $1 \leqslant n \leqslant N-2$ and $d_{N-1} \neq \pm 1$ is completely controllable since $v_1 = 1$, $v_n = 0$ for $2 \leqslant n \leqslant N-3$, $v_{N-2} = 1 - d_{N-1}^2$ and $v_{N-1} = 2d_{N-1}^2 - 1 \neq 0$, i.e., $v_1 \neq v_n$ for $n > 1$.

4. Limits of complete controllability

The theorems and corollaries in section 3 suggest that many non-decomposable quantum systems are completely controllable and one might actually begin to wonder if there are any non-decomposable (i.e., non-decoupled) systems that are not completely controllable. Unfortunately, the answer is yes, and worse yet, these systems may look very similar to completely controllable systems. Recall example 6, i.e., a system with energy levels (9), which satisfies the conditions for complete controllability of theorem 2 if the transition dipole moments are chosen as in (10) but does not satisfy the criteria for complete controllability if the d_n are chosen as in (11). We shall see that for the latter choice of the transition dipole moments d_n the system is indeed *not* completely controllable.

Theorem 4. *The dynamical Lie algebra for a system with N equally spaced energy levels $\mu_n = \mu$ for $1 \leqslant n \leqslant N-1$ and $v_n = v$ for $1 \leqslant n \leqslant N-1$ has dimension four, i.e., the system is not completely controllable for $N > 2$.*

Proof. Let $Y = \mathrm{i}H_1$,

$$X \equiv \mu^{-1}[\mathrm{i}H_0, Y] = \sum_{n=1}^{N-1} d_n x_{n,n+1}$$

$$Z \equiv 2^{-1}[X, Y] = \mathrm{i}\sum_{n=1}^{N} (d_n^2 - d_{n-1}^2) e_{nn}$$

and note that we have the following commutation relations

$$[\mathrm{i}H_0, X] = \mu Y \qquad [\mathrm{i}H_0, Y] = -\mu X \qquad [\mathrm{i}H_0, Z] = 0$$
$$[X, Y] = 2Z \qquad [Z, X] = -v_1 Y \qquad [Z, Y] = v_1 X.$$

Hence, $\mathrm{i}H_0, X, Y, Z$ span the Lie algebra $\mathcal{L}$. Thus $\mathcal{L}$ is isomorphic to the four-dimensional Lie algebra $u(2)$, i.e., the system is not completely controllable for $N > 2$. □

Example 9. If $N = 3$ and $\mu_1 = \mu_2$ as well as $d_1 = d_2$ then the system is not completely controllable since $v_1 = 2d_1^2 - d_2^2 = 2d_2^2 - d_1^2 = v_2$, i.e., the Lie algebra has dimension four according to the previous theorem.

Theorem 4 has another important implication. One can prove by induction that for $N > 4$ the condition $v_n = v$ for $1 \leqslant n \leqslant N-1$ can only be satisfied if

$$d_n^2 = nd_1^2 - \frac{n(n-1)}{2}v \qquad \text{and} \qquad v = \frac{2}{N-4}d_1^2.$$

Note that $v \to 0$ and thus $d_n \to nd_1^2$ for $N \to \infty$. Hence, the infinite-dimensional harmonic oscillator with $d_n = \sqrt{n}$ for $1 \leqslant n \leqslant \infty$ is *not* completely controllable.

Theorem 5. *A system with N equally spaced energy levels and $d_n = 1$ for $1 \leqslant n \leqslant N-1$ is not completely controllable for $N > 2$.*

Proof. Note that theorem 3 does not apply since $v_1 = v_{N-1} = 1$ and $v_2 = \cdots = v_{N-2} = 0$. Setting

$$Z_1 = \mathrm{i}(e_{11} - e_{nn})$$
$$X_1 = \mu^{-1}[\mathrm{i}H_0, \mathrm{i}H_1] = \sum_{n=1}^{N-1} x_{n,n+1}$$

leads to $[Z_1, X_1] = y_{12} + y_{N-1,N} \in \mathcal{L}$. Thus, we have the following reduced problem:

$$\mathrm{i}H_0 \qquad \mathrm{i}H_1^{(1)} = \mathrm{i}H_1 - [Z_1, X_1] = \sum_{n=2}^{N-2} y_{n,n+1}$$

and we can use induction to prove the theorem. One can easily verify that the system is not completely controllable if $N = 3$ (see example 9) or $N = 4$ (see section 5.1). Suppose the theorem is true for $N > 2$. We want to prove it is also true for $N + 2$. To this end, assume that the theorem is not true, i.e., that the $(N + 2)$-level system is completely controllable. Then we can use the above procedure to reduce the system to an N-level system. Clearly, this reduced N-level system must be completely controllable, which contradicts the assumption. This means that the assumption is false. □

5. Classification of complete controllability for four-level systems

In this section we apply the results of sections 3 and 4 to give a classification of the complete controllability problem for four-level quantum systems whose interaction with the control field is determined by (4).

According to theorem 2 and its corollaries, a non-decomposable four-level quantum system is completely controllable if $\mathrm{Tr}(H_0) \neq 0$ and one of the following conditions apply:

(i) $\mu_1 \neq \mu_2 \neq \mu_3$;
(ii) $\mu_1 \neq \mu_2 = \mu_3$;
(iii) $\mu_1 = \mu_2 \neq \mu_3$; or
(iv) $\mu_1 = \mu_3 \neq \mu_2$, $\mu_2 \neq 0$ and $d_1 \neq \pm d_3$.

Furthermore, if $\mu_1 = \mu_2 = \mu_3 \neq 0$ then the system is completely controllable according to theorem 3 if either

(i) $v_1 \neq v_2$, $v_1 \neq v_3$; or
(ii) $v_3 \neq v_1$, $v_3 \neq v_2$.

Decomposable systems (and traceless systems) are not completely controllable. Hence, the only cases that remain to be considered are the following.

5.1. Case $\mu_1 = \mu_3 \neq \mu_2$, $\mu_2 \neq 0$, $d_1 = \pm d_3$

In this case the system is *not* completely controllable and we actually have an 11-dimensional Lie algebra isomorphic to $sp(2) \oplus u(1)$. To see this, note that $sp(2)$ is spanned by [6]

$$\begin{aligned}
&h_1 \equiv \mathrm{i}(e_{11} - e_{33}) && h_2 \equiv \mathrm{i}(e_{22} - e_{44}) \\
&x_{2\omega_1} \equiv x_{31} && y_{2\omega_1} \equiv y_{31} \\
&x_{2\omega_2} \equiv x_{42} && y_{2\omega_2} \equiv y_{42} \\
&x_{\omega_1+\omega_2} \equiv x_{32} + x_{41} && y_{\omega_1+\omega_2} \equiv y_{32} + y_{41} \\
&x_{\omega_1-\omega_2} \equiv x_{21} - x_{34} && y_{\omega_1-\omega_2} \equiv y_{21} - y_{34}
\end{aligned} \qquad (13)$$

and if $d_1 = \pm d_3$ then the change of basis

$$\{|1\rangle, |2\rangle, |3\rangle, |4\rangle\} \mapsto \{|2\rangle, |1\rangle, |3\rangle, \mp|4\rangle\}$$

leads to

$$H_0 = \tfrac{1}{4}\,\mathrm{Tr}(H_0)I - (\mu_1 + \mu_2/2)h_1 + \mu_2 h_2$$
$$H_1 = d_1 y_{\omega_1-\omega_2} + d_2 y_{2\omega_1}$$

and one can easily check that $H_0' = \mu_1 h_1 + \mu_2 h_2$ and H_1 generate all of $sp(2)$. Hence, $\mathcal{L} \simeq sp(2) \oplus u(1)$.

5.2. *Case* $\mu_1 = \mu_3 \neq \mu_2$, $\mu_2 = 0$

$$X_1 \equiv \mu_1^{-1}[\mathrm{i}H_0, \mathrm{i}H_1] = d_1 x_{12} + d_3 x_{34}$$
$$Y_1 \equiv \mu_1^{-1}[\mathrm{i}H_0, X_1] = d_1 y_{12} + d_3 y_{34}$$
$$Z_1 \equiv 2^{-2}[X_1, Y_1] = \mathrm{i}[d_1^2(e_{11} - e_{22}) + d_3^2(e_{33} - e_{44})].$$

Then we have

$$Y_2 \equiv d_2^{-1}(\mathrm{i}Z_1 - Y_1) = y_{23} \in \mathcal{L}$$
$$X_2 \equiv (d_1^2 + d_2^2)^{-1}[Z_1, Y_2] = x_{23} \in \mathcal{L}.$$

According to lemma 2, the system is completely controllable if $d_1 \neq \pm d_3$. For $d_1 = \pm d_3$, the Lie algebra generated is the 11-dimensional Lie algebra given in the previous section, i.e., the system is not completely controllable.

5.3. *Case* $\mu_1 = \mu_2 = \mu_3$, $v_1 = v_3$, $v_2 \neq v_1$

From the definition of v_n we obtain that the condition $v_2 \neq v_1 = v_3$ is equivalent to $d_2^2 \neq d_1^2 = d_3^2$, which implies $d_1 = \pm d_3$. One can easily verify that $\mathcal{L}$ is the 11-dimensional algebra given in section 5.1. Hence, the system is not completely controllable.

5.4. *Case* $\mu_1 = \mu_2 = \mu_3$, $v_1 = v_2 = v_3$

In this case one can easily verify that $\mathrm{i}H_0$ and $\mathrm{i}H_1$ generate a Lie algebra of dimension four isomorphic to $u(2)$. Hence, the system is not completely controllable. Note that $v_1 = v_2 = v_3$ is equivalent to $d_3^2 = d_1^2 = \frac{3}{4}d_2^2$. (See also theorem 5.)

5.5. *Case* $\mu_1 = \mu_2 = \mu_3 = 0$

This is a completely degenerate system ($E_1 = E_2 = E_3 = E_4$) and $\mathcal{L}$ is a two-dimensional Lie algebra with basis $\mathrm{i}H_0 = \mathrm{i}I$ and $\mathrm{i}H_1$. Clearly, the system is not completely controllable.

6. Conclusion

In this paper we studied the problem of complete controllability of finite-level non-decomposable quantum systems whose interaction with a semi-classical field is governed by the dipole approximation. We reduced the problem of complete controllability of these systems to the question whether a pair of skew-Hermitian matrices $x_{n\,n+1}$ and $y_{n\,n+1}$ can be generated by $\mathrm{i}H_0$ and $\mathrm{i}H_1$. Using these criteria, we showed that many non-decomposable finite-level quantum systems are completely controllable, including many atomic systems as well as Morse and harmonic oscillator systems. We also showed, however, that complete controllability is by no means a universal property of the types of systems under consideration and that in fact many systems lacking complete controllability may appear superficially very similar to completely controllable ones. Finally, we applied our results to give a classification of four-level systems in terms of complete controllability, as presented in table 1.

Table 1. Complete controllability for four-level harmonic and anharmonic oscillator systems.

System	μ_n	$d_n (\neq 0)$	Complete controllability
Anharmonic	$\mu_1 \neq \mu_2 \neq \mu_3$		Yes
	$\mu_1 \neq \mu_2 = \mu_3$		Yes
	$\mu_1 = \mu_2 \neq \mu_3$		Yes
	$\mu_1 = \mu_3 \neq \mu_2$	$d_1 \neq d_3$	Yes
		$d_1 = d_3$	No
Harmonic	$\mu_1 = \mu_3 = \mu_3 \neq 0$	$v_1 \neq v_2 \neq v_3$	Yes
		$v_1 \neq v_2 = v_3$	Yes
		$v_1 = v_2 \neq v_3$	Yes
		$v_1 = v_3 \neq v_2, d_1 = \pm d_3$	No
		$v_1 = v_2 = v_3$	No
	$\mu_1 = \mu_3 = \mu_3 = 0$		No

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