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Identification of dynamical Lie algebras for finite-level quantum control systems

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Abstract

The problem of identifying the dynamical Lie algebras of finite-level quantum systems subject to external control is considered, with special emphasis on systems that are not completely controllable. In particular, it is shown that the dynamical Lie algebra for an N-level system with symmetrically coupled transitions, such as a system with equally spaced energy levels and uniform transition dipole moments, is a subalgebra of $so(N)$ if $N = 2\ell + 1$, and a subalgebra of $sp(\ell)$ if $N = 2\ell$. General criteria for obtaining either $so(2\ell + 1)$ or $sp(\ell)$ are established.

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1. Introduction

In [1] we studied the problem of complete controllability of finite-level quantum systems with nearest-neighbour interactions. We showed that many quantum systems of physical interest are indeed completely controllable but that there are nevertheless systems with certain symmetries that are not completely controllable. This paper is devoted to identifying the dynamical Lie algebras for the latter systems.

As in the previous paper, we consider the case of a driven quantum system, for which the interaction with the control field is linear, i.e., we assume that the total Hamiltonian of the system is

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

where H_0 is the internal system Hamiltonian and H_1 represents the interaction of the system with the real control field f. We assume that H_0 and H_1 are Hermitian. 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 the internal Hamiltonian can be expanded in terms of the energy eigenfunctions $|n\rangle$,

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

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 since H_0 is Hermitian. We shall assume that the energy levels are ordered in a non-decreasing sequence, i.e., $E_1 \leqslant E_2 \leqslant \ldots \leqslant E_N$. Hence, the frequencies for transitions $|n\rangle \rightarrow |n+1\rangle$ are non-negative

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

In the following it will be convenient to deal with trace-zero operators. Thus, if H_0 has non-zero trace then we define the trace-zero operator

$$H_0' = H_0 - \left[N^{-1}\,\mathrm{Tr}(H_0)\right] I_N \tag{4}$$

which is equivalent to H_0 up to the addition of a constant multiple of the identity matrix I_N. Expanding the interaction Hamiltonian H_1 with respect to the 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 the transition dipole moments $d_{m,n}$, which we assume real, satisfy $d_{m,n} = d_{n,m}$. In this paper we shall only be concerned with quantum systems for which the interaction with the control field is determined by transitions between adjacent energy levels, as is typical in the dipole approximation. It will also be assumed that there are no 'self-interactions', i.e., that the diagonal elements $d_{n,n}$ are zero for all n. Thus, letting $d_n = d_{n,n+1}$ for $1 \leqslant n \leqslant N-1$ we have

$$H_1 = \sum_{n=1}^{N-1} d_n(|n\rangle\langle n+1| + |n+1\rangle\langle n|) = \sum_{n=1}^{N-1} d_n(e_{n,n+1} + e_{n+1,n}). \tag{5}$$

2. Dynamical Lie algebras

The operators $\mathrm{i}H_0$ and $\mathrm{i}H_1$ generate a Lie algebra $\mathcal{L}$ called the dynamical Lie algebra of the control system. This Lie algebra is important since it determines the Lie group S on which the control system evolves [2]. Precisely speaking, the trajectories of the system subject to any control field are confined to the exponential image of the Lie algebra $\mathcal{L}$. Knowledge of the dynamical Lie algebra thus enables us to determine the degree of controllability of a quantum system [3, 4], to identify reachable or non-reachable target states [5, 6], and to determine whether a kinematical bound for an observable is dynamically accessible [7, 8].

The dynamical Lie algebra $\mathcal{L}$ generated by the operators $\mathrm{i}H_0$ and $\mathrm{i}H_1$ defined in (2) and (5) is a real Lie algebra of $N \times N$ skew-Hermitian matrices, and the related Lie algebra $\mathcal{L}'$ generated by $\mathrm{i}H_0'$ and $\mathrm{i}H_1$ is a real Lie algebra of traceless, skew-Hermitian matrices. Thus, $\mathcal{L}'$ is always a subalgebra of $su(N)$. Since $\mathcal{L}$ is isomorphic to $\mathcal{L}' \oplus u(1)$ if $\mathrm{Tr}(H_0) \neq 0$ and $\mathcal{L} = \mathcal{L}'$ if $\mathrm{Tr}(H_0) = 0$, it suffices to determine $\mathcal{L}'$. It follows from classical results that a pair of skew-Hermitian matrices in $su(N)$ almost always generates the full Lie algebra $su(N)$ (see lemma 4 in [9], for example). For the type of quantum systems considered in this paper, explicit criteria ensuring $\mathcal{L}' = su(N)$ have been established [1]:

Theorem 1. *Let $d_0 = d_N = 0$ and $v_m = 2d_m^2 - d_{m+1}^2 - d_{m-1}^2$ for $1 \leqslant m \leqslant N-1$. The dynamical Lie algebra $\mathcal{L}'$ generated by $\mathrm{i}H_0'$ and $\mathrm{i}H_1$ defined in (4) and (5) is $su(N)$ if $d_m \neq 0$, $E_m \neq 0$ for $1 \leqslant m \leqslant N-1$, and one of the following criteria applies:*

(i) there exists $\mu_p \neq 0$ such that $\mu_m \neq \mu_p$ for $m \neq p$, or
(ii) $\mu_m = \mu$ for $1 \leqslant m \leqslant N-1$ but there exists $v_p \neq 0$ such that $v_m \neq v_p$ for $m \neq p$.

If $p = \frac{1}{2}N$ then $d_{p-k} \neq \pm d_{p+k}$ for some $k > 0$ is required as well.

As has been shown in [1], many quantum systems of physical interest indeed satisfy these criteria. However, there are systems of physical interest that do not meet these criteria. For instance, if any of the dipole moments d_n vanish then the system decomposes into independent subsystems and its dynamical Lie algebra $\mathcal{L}'$ is a sum of subalgebras of $su(N)$ [8]. But even if all the d_n are non-zero, the dynamical Lie algebra of the system may be a proper subalgebra of $su(N)$, for example, if the transition frequencies μ_n and the transition dipole moments d_n satisfy

$$\mu_n = \mu_{N-n} \qquad d_n = d_{N-n} \qquad 1 \leqslant n \leqslant N-1 \tag{6}$$

as is the case for a system with N equally spaced energy levels and uniform dipole moments. In the following we show that the dynamical Lie algebra $\mathcal{L}'$ of such a system is a subalgebra of $so(2\ell+1)$ if $N = 2\ell+1$, and a subalgebra of $sp(\ell)$ if $N = 2\ell$, and give criteria ensuring $\mathcal{L}' = so(2\ell+1)$ or $\mathcal{L}' = sp(\ell)$, respectively. In appendix D, we also briefly discuss why the Lie algebra $so(2\ell)$ does not arise for the systems considered in this paper.

3. The case $N = 2\ell + 1$: dynamical Lie algebra $so(2\ell + 1)$

Consider a system with Hamiltonian $H = H_0 + f(t)H_1$, where

$$\mathrm{i}H_0 = \sum_{n=1}^{2\ell+1} E_n \mathrm{i} e_{n,n} \qquad \mathrm{i}H_1 = \sum_{n=1}^{2\ell} d_n \mathrm{i}(e_{n,n+1} + e_{n+1,n}) \tag{7}$$

$E_1 \leqslant E_2 \leqslant \ldots E_N$, $E_1 \neq E_N$, $d_n \neq 0$ for all n, and the transition frequencies $\mu_n = E_{n+1} - E_n$ and transition dipole moments d_n satisfy the symmetry relation (6). We shall prove that the Lie algebra $\mathcal{L}'$ is a subalgebra of $so(2\ell+1)$, which is in general isomorphic to $so(2\ell+1)$.

3.1. $\mathcal{L}' \subseteq so(2\ell + 1)$

We show first that $\mathcal{L}' \subseteq so(2\ell+1)$. Let $y_{n,m} = \mathrm{i}(e_{n,m} + e_{m,n})$. Using $d_n = d_{2\ell+1-n}$ and $y_{m,n} = y_{n,m}$ we can simplify $\mathrm{i}H_1$,

$$\mathrm{i}H_1 = \sum_{n=1}^{\ell} d_{\ell+1-n}(y_{\ell+2-n,\ell+1-n} + y_{\ell+n,\ell+n+1}).$$

To compute H_0', we note that $E_n = E_1 + \sum_{s=1}^{n-1} \mu_s$. Thus, using $\mu_n = \mu_{2\ell+1-n}$ leads to

$$\mathrm{Tr}(H_0) = (2\ell+1)E_1 + (2\ell+1)\sum_{s=1}^{\ell} \mu_s.$$

Hence, the energy levels E_n' of H_0' are $E_{\ell+1}' = 0$ and

$$E_{\ell+1-n}' = -\sum_{s=\ell+1-n}^{\ell} \mu_s \qquad E_{\ell+1+n}' = \sum_{s=\ell+1}^{\ell+n} \mu_s = \sum_{s=\ell+1-n}^{\ell} \mu_s$$

for $1 \leqslant n \leqslant \ell$. Consequently, we have

$$\mathrm{i}H_0' = \sum_{n=1}^{\ell} \left(- \sum_{s=\ell+1-n}^{\ell} \mu_s \right) \mathrm{i}(e_{\ell+1-n,\ell+1-n} - e_{\ell+1+n,\ell+1+n}).$$

Let σ be an isomorphism of the Hilbert space of pure states defined by

$$\sigma(|n\rangle) = \begin{cases} |\ell+2-n\rangle & 1 \leqslant n \leqslant \ell+1 \\ (-1)^{n-\ell-1}|n\rangle & \ell+2 \leqslant n \leqslant 2\ell+1 \end{cases} \tag{8}$$

and set $|m\rangle = \sigma(|n\rangle)$ as well as $\tilde{E}_m = -\sum_{s=\ell+1-m}^{\ell} \mu_s$ and $\tilde{d}_m = d_{\ell+1-m}$. Then the representations of $\mathrm{i}H_0'$ and $\mathrm{i}H_1$ with respect to the new basis $|m\rangle$ are

$$\begin{aligned} \mathrm{i}H_0' &= \sum_{m=1}^{\ell} \left(- \sum_{s=\ell+1-m}^{\ell} \mu_s \right) \mathrm{i}(e_{m+1,m+1} - e_{\ell+1+m,\ell+1+m}) = \sum_{m=1}^{\ell} \tilde{E}_m h_m \\ \mathrm{i}H_1 &= d_\ell(y_{1,2} + y_{1,\ell+2}) + \sum_{m=2}^{\ell} d_{\ell+1-m}(y_{m,m+1} - y_{m+\ell,m+\ell+1}) = \sum_{m=1}^{\ell} \tilde{d}_m y_m \end{aligned} \tag{9}$$

with h_m and y_m as defined in (B.1) and (B.3), respectively. Hence, $\mathrm{i}H_0'$ and $\mathrm{i}H_1$ are both in $so(2\ell+1)$ and thus the Lie algebra $\mathcal{L}'$ they generate must be contained in $so(2\ell+1)$.

Since $\mathrm{i}H_0'$ and $\mathrm{i}H_1$ in (9) contain a complete set of generators h_m and y_m for $so(2\ell+1)$ (see appendix B), it is natural to expect that they generate the full Lie algebra $so(2\ell+1)$. We shall prove that this is usually, but not inevitably, true.

Example 1. Consider a system of type (7) for $\ell = 3$. If $E_m = m$, $1 \leqslant m \leqslant 7$ and $d_1 = d_6 = \sqrt{3}$, $d_2 = d_5 = \sqrt{5}$ and $d_3 = d_4 = \sqrt{6}$ then the basis change (8) leads to

$$\mathrm{i}H_0' = -h_1 - 2h_2 - 3h_3 \qquad \mathrm{i}H_1 = \sqrt{6}y_1 + \sqrt{5}y_2 + \sqrt{3}y_3$$

with h_m and y_m as defined in (B.1) and (B.3), respectively. Therefore, the Lie algebra $\mathcal{L}'$ generated by $\mathrm{i}H_0'$ and $\mathrm{i}H_1$ is a subalgebra of $so(7)$. However, it is easy to verify that $\mathcal{L}' \not\simeq so(7)$. Indeed, in this particular case $\mathcal{L}'$ is a three-dimensional subalgebra of $so(7)$ spanned by $\mathrm{i}H_0$, $\mathrm{i}H_1$ and $[\mathrm{i}H_0, \mathrm{i}H_1] = \sqrt{6}x_1 + \sqrt{5}x_2 + \sqrt{3}x_3$.

Thus, for certain choices of the parameters E_m and d_m, the Lie algebra $\mathcal{L}'$ is a *proper* subalgebra of $so(2\ell+1)$.

3.2. Criteria for $\mathcal{L}' = so(2\ell+1)$

To find criteria that ensure $\mathcal{L}' = so(2\ell+1)$, consider the generic system

$$\mathrm{i}H_0' = \sum_{m=1}^{\ell} \epsilon_m h_m \qquad \mathrm{i}H_1 = \sum_{m=1}^{\ell} \delta_m y_m \qquad \epsilon_m \neq 0 \quad \delta_m \neq 0 \quad \forall m \tag{10}$$

with h_m and y_m as defined in (B.1) and (B.3), respectively. As before, $\mathrm{i}H_0$ and $\mathrm{i}H_1$ are in $so(2\ell+1)$ and hence the Lie algebra $\mathcal{L}'$ they generate must be contained in $so(2\ell+1)$.

Theorem 2. *Let $\omega_m = \epsilon_{m+1} - \epsilon_m$ for $1 \leqslant m < \ell$ and $\omega_0 = \epsilon_1$. The dynamical Lie algebra $\mathcal{L}'$ generated by the system $H = H_0' + f(t)H_1$ with $\mathrm{i}H_0'$ and $\mathrm{i}H_1$ as in (10) is $so(2\ell+1)$ if $\omega_m^2 \neq \omega_0^2$ for $1 \leqslant m \leqslant \ell$.*

Proof. Using the properties of the generators h_m and y_m leads to

$$\begin{aligned}
V^{(0)} &\equiv [[\mathrm{i}H_0', \mathrm{i}H_1], \mathrm{i}H_0'] \\
&= \sum_{m=1}^{\ell} \delta_m \omega_{m-1}^2 y_m \\
V^{(1)} &\equiv \left[\left[\mathrm{i}H_0', V^{(0)}\right], \mathrm{i}H_0'\right] - \omega_{\ell-1}^2 V^{(0)} \\
&= \sum_{m=1}^{\ell-1} \delta_m \omega_{m-1}^2 \left(\omega_{m-1}^2 - \omega_{\ell-1}^2\right) y_m \\
V^{(2)} &\equiv \left[\left[\mathrm{i}H_0', V^{(1)}\right], \mathrm{i}H_0'\right] - \omega_{\ell-2}^2 V^{(1)} \\
&= \sum_{m=1}^{\ell-2} \delta_m \omega_{m-1}^2 \left(\omega_{m-1}^2 - \omega_{\ell-1}^2\right)\left(\omega_{m-1}^2 - \omega_{\ell-2}^2\right) y_m \\
&\vdots \\
V^{(\ell-1)} &\equiv \left[\left[\mathrm{i}H_0', V^{(\ell-2)}\right], \mathrm{i}H_0'\right] - \omega_1^2 V^{(\ell-2)} \\
&= \delta_1 \omega_0^2 \prod_{m=1}^{\ell-1} \left(\omega_0^2 - \omega_m^2\right) y_1.
\end{aligned}$$

By hypothesis $\omega_m^2 \neq \omega_0^2$ for $m > 0$ and $\delta_1 \neq 0$, $\omega_0 = \epsilon_1 \neq 0$. Hence, all the factors in the last expression above are non-zero, i.e., we have $y_1 \in \mathcal{L}'$ and thus $\mathcal{L}' = so(2\ell+1)$ by lemma 1 of appendix B. □

If $\omega_m^2 = \omega_0^2$ for some $m > 0$ then a slight modification of the proof above leads to a residual term

$$Y^{(0)} \equiv \sum_{m \in \mathcal{M}} \delta_m y_m = \sum_{m=1}^{\ell} \tilde{\delta}_m y_m \tag{11}$$

where $\mathcal{M} = \left\{m : 1 \leqslant m \leqslant \ell, \omega_{m-1}^2 = \omega_0^2\right\}$ with $\tilde{\delta}_m = \delta_m$ for $m \in \mathcal{M}$ and $\tilde{\delta}_m = 0$ otherwise. If the energy levels are either positive and ordered in a non-decreasing sequence, i.e., $0 \leqslant \epsilon_m \leqslant \epsilon_{m+1}$, or negative and ordered in a non-increasing sequence, i.e., $0 \geqslant \epsilon_m \geqslant \epsilon_{m+1}$, then $\omega_{m-1}^2 = \omega_0^2$ implies $\omega_{m-1} = \omega_0$ for all $m \in \mathcal{M}$. We shall only consider this case in the following.

Theorem 3. *Let* $v_m \equiv 2\tilde{\delta}_m^2 - \tilde{\delta}_{m+1}^2 - \tilde{\delta}_{m-1}^2$ *for* $1 \leqslant m \leqslant \ell$, *where* $\tilde{\delta}_0 = \tilde{\delta}_1$, $\tilde{\delta}_{\ell+1} = 0$. *The dynamical Lie algebra* $\mathcal{L}'$ *generated by the system* $H = H_0' + f(t)H_1$ *with* $\mathrm{i}H_0'$ *and* $\mathrm{i}H_1$ *as in (10) is* $so(2\ell+1)$ *if* $\omega_{m-1} = \omega_0$ *but* $v_m \neq v_1$ *for all* $m \in \mathcal{M} - \{1\}$.

Proof. Since $\omega_{m-1} = \omega_0$ for all $m \in \mathcal{M}$, we have

$$\begin{aligned}
X^{(0)} &\equiv \omega_0^{-1}\left[\mathrm{i}H_0', Y^{(0)}\right] \\
Z &\equiv 2^{-1}\left[X^{(0)}, Y^{(0)}\right] = \sum_{m=1}^{\ell} \left(\tilde{\delta}_{m+1}^2 - \tilde{\delta}_m^2\right) h_m.
\end{aligned}$$

Suppose $\mathcal{M} - \{1\}$ has ℓ' elements labelled m_1, m_2 up to $m_{\ell'}$. If $v_m \neq v_1$ for all $m \in \mathcal{M} - \{1\}$ then

$$
\begin{aligned}
Y^{(1)} &\equiv \left[Z, X^{(0)}\right] - v_{m_{\ell'}} Y^{(0)} \\
&= \tilde{\delta}_1 \left(v_1 - v_{m_{\ell'}}\right) y_1 - \sum_{k=1}^{\ell'-1} \tilde{\delta}_{m_k} \left(v_{m_k} - v_{m_{\ell'}}\right) y_{m_k} \\
X^{(1)} &\equiv \left[Y^{(0)}, Z\right] - v_{m_{\ell'}} X^{(0)} \\
&= \tilde{\delta}_1 \left(v_1 - v_{m_{\ell'}}\right) x_1 - \sum_{k=1}^{\ell'-1} \tilde{\delta}_{m_k} \left(v_{m_k} - v_{m_{\ell'}}\right) x_{m_k} \\
Y^{(2)} &\equiv \left[Z, X^{(1)}\right] - v_{m_{\ell'-1}} Y^{(1)} \\
&= \tilde{\delta}_1 \left(v_1 - v_{m_{\ell'}}\right)\left(v_1 - v_{m_{\ell'-1}}\right) y_1 - \sum_{k=1}^{\ell'-2} \tilde{\delta}_{m_k} \left(v_{m_k} - v_{m_{\ell'}}\right)\left(v_{m_k} - v_{m_{\ell'-1}}\right) y_{m_k} \\
X^{(2)} &\equiv \left[Y^{(1)}, Z\right] - v_{m_{\ell'-1}} X^{(1)} \\
&= \tilde{\delta}_1 \left(v_1 - v_{m_{\ell'}}\right)\left(v_1 - v_{m_{\ell'-1}}\right) x_1 - \sum_{k=1}^{\ell'-2} \tilde{\delta}_{m_k} \left(v_{m_k} - v_{m_{\ell'}}\right)\left(v_{m_k} - v_{m_{\ell'-1}}\right) x_{m_k} \\
&\vdots \\
Y^{(\ell')} &\equiv \tilde{\delta}_1 \prod_{k=1}^{\ell'} \left(v_1 - v_{m_k}\right) y_1
\end{aligned}
$$

shows that $y_1 \in \mathcal{L}'$ and hence $\mathcal{L}' = so(2\ell + 1)$ by lemma 1 of appendix B. □

A similar argument shows that if there exists $k \in M$ such that $v_m \neq v_k$ for $m \in \mathcal{M} \cup \{1\}$ but $m \neq k$, then $y_k \in \mathcal{L}'$. Using the fact that the generators y_m of $so(2\ell + 1)$ are not diagonal with respect to the Cartan elements (see appendix B), it generally follows that $\mathcal{L}'$ contains all the generators x_m and y_m and thus $\mathcal{L}' = so(2\ell + 1)$ as well. An important special case of this type is a system with $N = 2\ell + 1$ equally spaced energy levels and uniform transition dipole moments.

Theorem 4. *The dynamical Lie algebra $\mathcal{L}'$ generated by the system $H = H_0' + f(t)H_1$ with $N = 2\ell + 1$ equally spaced energy levels $\omega_m = \epsilon_1$ and uniform dipole moments $\delta_m = \delta$ is $so(2\ell + 1)$.*

Proof. Let $Y^{(1)} = \delta^{-1}\mathrm{i}H_1$ and $X^{(1)} = \epsilon_1^{-1}\left[\mathrm{i}H_0', Y^{(1)}\right]$. Then $h_\ell = -2^{-1}\left[X^{(1)}, Y^{(1)}\right]$, $y_\ell = \left[h_\ell, X^{(1)}\right]$ and $x_\ell = [y_\ell, h_\ell]$. Thus, $x_\ell,\ y_\ell \in \mathcal{L}'$. Next, set $Y^{(k+1)} = Y^{(k)} - y_{\ell+1-k}$ and $X^{(k+1)} = X^{(k)} - x_{\ell+1-k}$ for $1 \leqslant k < \ell$, and note that $h_{\ell-k} = 2^{-1}\left[Y^{(k+1)}, X^{(k+1)}\right]$, $y_{\ell-k} = \left[h_{\ell-k}, X^{(k+1)}\right]$ and $x_{\ell-k} = [y_{\ell-k}, h_{\ell-k}]$. This shows that $\mathcal{L}'$ contains all the generators x_m and y_m of $so(2\ell + 1)$. Hence, $\mathcal{L}' = so(2\ell + 1)$. □

3.3. Application of the criteria

We shall now return to the original system (7). Since we have assumed that the energy levels are ordered in a non-decreasing sequence, we have $\mu_m \geqslant 0$ for all m and hence

$$
\tilde{E}_m = -\sum_{s=\ell+1-m}^{\ell} \mu_s \leqslant 0 \qquad \tilde{E}_m \geqslant \tilde{E}_{m+1} \qquad 1 \leqslant m \leqslant \ell
$$

i.e., the energy levels $\tilde{E}_m$ are negative and form a decreasing (non-increasing) sequence. Noting that $\epsilon_m = \tilde{E}_m$, we thus have $\omega_0 = \epsilon_1 = \tilde{E}_1 = -\mu_{\ell+1} \leqslant 0$ and

$$\omega_m = \epsilon_{m+1} - \epsilon_m = \tilde{E}_{m+1} - \tilde{E}_m = \sum_{s=\ell-m+1}^{\ell} \mu_s - \sum_{\ell-m}^{\ell} \mu_s = -\mu_{\ell-m+1} \leqslant 0.$$

If $\mu_\ell \neq 0$ and $\mu_m \neq \mu_\ell$ for $m < \ell$ then $\mathcal{L}' = so(2\ell+1)$ according to theorem 2, independent of the choice of the dipole moments, provided that they are non-zero.

If $\mu_m = \mu_\ell$ for some $m < \ell$ then theorem 3 applies and the dipole moments determine whether we have $\mathcal{L}' = so(2\ell+1)$ or a proper subalgebra. In particular, the Lie algebra is $so(2\ell+1)$ if the energy levels are equally spaced, $\mu_m = \mu_\ell$ for all m, and the dipole moments d_m are such that $v_m \neq v_1$ for all $m > 1$, where

$$v_m = 2\tilde{d}_m^2 - \tilde{d}_{m-1}^2 - \tilde{d}_{m+1}^2 = 2d_{\ell+1-m}^2 - d_{\ell+2-m}^2 - d_{\ell-m}^2$$

for $1 < m \leqslant \ell$ and $v_1 = \tilde{d}_1^2 - \tilde{d}_2^2 = d_\ell^2 - d_{\ell-1}^2$ (with $d_0 = 0$). For instance, setting $d_m = \sqrt{m}$ for $1 \leqslant m \leqslant \ell$ works since it gives $v_1 = \ell - (\ell-1) = 1$ but $v_m = 2(\ell+1-m) - (\ell+2-m) - (\ell-m) = 0$ for $m > 1$. Setting $d_m = 1$ also gives $\mathcal{L}' = so(2\ell+1)$ due to theorem 4.

However, recall that there are systems of type (7) whose Lie algebra $\mathcal{L}'$ is a proper subalgebra of $so(2\ell+1)$, as example 1 above clearly shows. Note that in this example, the energy levels are equally spaced and the dipole moments d_m are such that $v_1 = 2d_3^2 - d_2^2 = 6 - 5 = 1$, $v_2 = 2d_2^2 - d_1^2 - d_3^2 = 2 \times 5 - 6 - 3 = 1$ and $v_3 = 2d_1^2 - d_2^2 = 2 \times 3 - 5 = 1$, i.e., all the v_m are equal and none of the theorems above are applicable.

4. The case $N = 2\ell$: dynamical Lie algebra $sp(\ell)$

Let $N = 2\ell$ and consider the system $H = H_0 + f(t)H_1$ with

$$\mathrm{i}H_0 = \sum_{n=1}^{2\ell} E_n \mathrm{i} e_{n,n} \qquad \mathrm{i}H_1 = \sum_{n=1}^{2\ell-1} d_n y_{n,n+1} \tag{12}$$

where $\mu_n = \mu_{2\ell-n}$ and $d_n = d_{2\ell-n}$ for $1 \leqslant n \leqslant \ell-1$. Note the symmetry of the system. Every transition frequency except μ_ℓ occurs in pairs, and although μ_ℓ may be different from all the other μ_n, theorem 1 does not apply since $N = 2\ell$ and there is no k such that $d_{\ell-k} \neq \pm d_{\ell+k}$. In fact, we shall prove that the Lie algebra generated by $\mathrm{i}H_0'$ and $\mathrm{i}H_1$ is a subalgebra of $sp(\ell)$, which is in general isomorphic to $sp(\ell)$.

4.1. $\mathcal{L}' \subseteq sp(\ell)$

To show that $\mathcal{L}' \subseteq sp(\ell)$, we note that $d_{2\ell-n} = d_n$ implies

$$\mathrm{i}H_1 = d_\ell y_{\ell,\ell+1} + \sum_{n=1}^{\ell-1} d_n (y_{n,n+1} + y_{2\ell-n,2\ell+1-n}).$$

Furthermore, $E_n = E_1 + \sum_{s=1}^{n-1} \mu_s$ and $\mu_{2\ell-n} = \mu_n$ for $1 \leqslant n \leqslant \ell-1$ leads to

$$\mathrm{Tr}(H_0) = (2\ell)E_1 + (2\ell)\sum_{s=1}^{\ell-1} \mu_s + \ell\mu_\ell.$$

Hence, $\mathrm{Tr}(H_0)/(2\ell) = E_1 + \sum_{s=1}^{\ell-1} \mu_s + \frac{1}{2}\mu_\ell$ and the energy levels E'_n of H'_0 are $E'_\ell = -\frac{1}{2}\mu_\ell$, $E'_{\ell+1} = \frac{1}{2}\mu_\ell$ and

$$E'_{\ell-n} = -\sum_{s=\ell-n}^{\ell-1} \mu_s - \frac{\mu_\ell}{2} \qquad E'_{\ell+1+n} = \sum_{s=\ell+1}^{\ell+n} \mu_s + \frac{\mu_\ell}{2} = \sum_{s=\ell-n}^{\ell-1} \mu_s + \frac{\mu_\ell}{2}$$

for $1 \leqslant n \leqslant \ell - 1$. Thus, we have

$$\mathrm{i}H'_0 = \sum_{n=1}^{\ell} -\left(\frac{\mu_\ell}{2} + \sum_{s=n}^{\ell-1} \mu_s\right) \mathrm{i}(e_{n,n} - e_{2\ell+1-n,2\ell+1-n}).$$

Let σ be an isomorphism of the Hilbert space of pure states defined by

$$\sigma(|n\rangle) = \begin{cases} |n\rangle & 1 \leqslant n \leqslant \ell \\ (-1)^{n-\ell-1}|3\ell+1-n\rangle & \ell+1 \leqslant n \leqslant 2\ell \end{cases} \tag{13}$$

and set $|m\rangle = \sigma(|n\rangle)$ as well as $\tilde{E}_m = -\frac{1}{2}\mu_\ell - \sum_{s=m}^{\ell-1} \mu_s$ for $1 \leqslant m \leqslant \ell - 1$, $\tilde{E}_\ell = -\frac{1}{2}\mu_\ell$, $\tilde{d}_\ell = d_\ell$. Then $\mathrm{i}H'_0$ and $\mathrm{i}H_1$ have the following representations with respect to the new basis $|m\rangle$

$$\begin{aligned} \mathrm{i}H'_0 &= \sum_{m=1}^{\ell} -\left(\frac{\mu_\ell}{2} + \sum_{s=m}^{\ell-1} \mu_s\right) \mathrm{i}(e_{m,m} - e_{m+\ell,m+\ell}) = \sum_{m=1}^{\ell} \tilde{E}_m h_m \\ \mathrm{i}H_1 &= d_\ell y_{\ell,2\ell} + \sum_{m=1}^{\ell-1} d_m (y_{m+1,m} - y_{m+\ell,m+\ell+1}) = \sum_{m=1}^{\ell} d_m y_m \end{aligned} \tag{14}$$

where h_m and y_m are as defined in (C.1) and (C.3), respectively, and we note that $y_{m,m+1} = y_{m+1,m}$, $y_{m+\ell,m+\ell+1} = y_{m+\ell+1,m+\ell}$. Hence, the dynamical Lie algebra generated by $\mathrm{i}H'_0$ and $\mathrm{i}H_1$ must be a subalgebra of $sp(\ell)$.

Since $\mathrm{i}H'_0$ and $\mathrm{i}H_1$ in (14) contain a complete set of generators h_m and y_m for $sp(\ell)$, it is natural to expect that they generate the full Lie algebra $sp(\ell)$. We shall prove that this is true in most cases. However, as in case of $so(2\ell+1)$, a proper subalgebra may also be generated.

Example 2. Consider a system of type (12) for $\ell = 3$. If $E_m = m$, $1 \leqslant m \leqslant 6$ and $d_1 = d_5 = \sqrt{5}$, $d_2 = d_4 = 2\sqrt{2}$ and $d_3 = 3$ then the basis change (13) leads to

$$\mathrm{i}H'_0 = -2.5h_1 - 1.5h_2 - 0.5h_3 \qquad \mathrm{i}H_1 = \sqrt{5}y_1 + 2\sqrt{2}y_2 + 3y_3$$

with h_m and y_m as defined in (C.1) and (C.3), respectively. Therefore, the Lie algebra $\mathcal{L}'$ generated by $\mathrm{i}H'_0$ and $\mathrm{i}H_1$ is a subalgebra of $sp(3)$. However, it is easy to verify that $\mathcal{L}' \not\simeq sp(3)$. Indeed, $\mathcal{L}'$ is a three-dimensional subalgebra of $sp(3)$ spanned by $\mathrm{i}H_0$, $\mathrm{i}H_1$ and $[\mathrm{i}H_0, \mathrm{i}H_1] = -(\sqrt{5}x_1 + 2\sqrt{2}x_2 + 3x_3)$.

Thus, for certain choices of the parameters E_m and d_m, the Lie algebra $\mathcal{L}'$ is a *proper* subalgebra of $sp(\ell)$.

4.2. Criteria for $\mathcal{L}' = sp(\ell)$

To find conditions that ensure $\mathcal{L}' = sp(\ell)$, we consider the generic system

$$\mathrm{i}H'_0 = \sum_{m=1}^{\ell} \epsilon_m h_m \qquad \mathrm{i}H_1 = \sum_{m=1}^{\ell} \delta_m y_m \qquad \epsilon_m \neq 0 \quad \delta_m \neq 0 \quad \forall m \tag{15}$$

with h_m and y_m as in (C.1) and (C.3). Clearly, $\mathrm{i}H'_0$ and $\mathrm{i}H_1$ are in $sp(\ell)$. Hence the Lie algebra $\mathcal{L}'$ they generate must be contained in $sp(\ell)$.

Theorem 5. *Let $\omega_m = \epsilon_{m+1} - \epsilon_m$ for $1 \leqslant m < \ell$ and $\omega_\ell = 2\epsilon_\ell$. The dynamical Lie algebra $\mathcal{L}'$ generated by $\mathrm{i}H_0'$ and $\mathrm{i}H_1$ as in (15) is $sp(\ell)$ if $\omega_m^2 \neq \omega_\ell^2$ for $m < \ell$.*

Proof. Using the properties of the generators h_m and y_m leads to:

$$\begin{aligned}
V^{(1)} &\equiv [[\mathrm{i}H_0', \mathrm{i}H_1], \mathrm{i}H_0'] - \omega_1^2(\mathrm{i}H_1) \\
&= \sum_{m=2}^{\ell} \delta_m \left(\omega_m^2 - \omega_1^2\right) y_m \\
V^{(2)} &\equiv \left[\left[\mathrm{i}H_0', V^{(1)}\right], \mathrm{i}H_0'\right] - \omega_2^2 V^{(1)} \\
&= \sum_{m=3}^{\ell} \delta_m \left(\omega_m^2 - \omega_1^2\right)\left(\omega_m^2 - \omega_2^2\right) y_m \\
&\vdots \\
V^{(\ell-1)} &\equiv \left[\left[\mathrm{i}H_0', V^{(\ell-2)}\right], \mathrm{i}H_0'\right] - \omega_{\ell-1}^2 V^{(\ell-2)} \\
&= \delta_\ell \prod_{m=1}^{\ell-1} \left(\omega_\ell^2 - \omega_m^2\right) y_\ell.
\end{aligned}$$

By hypothesis $\omega_m^2 \neq \omega_\ell^2$ for $m < \ell$ and $\delta_\ell \neq 0$. Hence, all the factors in the last expression above are non-zero, i.e., we have $y_\ell \in \mathcal{L}'$ and thus $\mathcal{L}' = sp(\ell)$ by lemma 2 of appendix C. □

If $\omega_m^2 = \omega_\ell^2$ for some $m < \ell$ then a modification of the proof above leads to a residual term

$$Y^{(0)} \equiv \sum_{m \in \mathcal{M}} \delta_m y_m = \sum_{m=1}^{\ell} \tilde{\delta}_m y_m$$

where $\mathcal{M} = \left\{m : 1 \leqslant m \leqslant \ell, \omega_m^2 = \omega_\ell^2\right\}$ and $\tilde{\delta}_m = \delta_m$ for $m \in \mathcal{M}$ and $\tilde{\delta}_m = 0$ otherwise.

If the energy levels ϵ are negative and ordered in an increasing (non-decreasing) sequence then $\omega_m^2 = \omega_\ell^2$ implies $\omega_m = -\omega_\ell = -2\epsilon_\ell \geqslant 0$ for all $m \in \mathcal{M}$. We shall only consider this case in the following.

Theorem 6. *Let $v_m = 2\tilde{\delta}_m^2 - \tilde{\delta}_{m+1}^2 - \tilde{\delta}_{m-1}^2$ for $1 \leqslant m \leqslant \ell$ and $\tilde{\delta}_{\ell+1} = \tilde{\delta}_{\ell-1}$, $\tilde{\delta}_0 = 0$. The dynamical Lie algebra $\mathcal{L}'$ generated by the system $H = H_0' + f(t)H_1$ with $\mathrm{i}H_0'$ and $\mathrm{i}H_1$ as in (15) is $sp(\ell)$ if $\mu_m = -\mu_\ell = -2\epsilon_\ell$ but $v_m \neq v_\ell$ for all $m \in \mathcal{M} - \{\ell\}$.*

Proof. Let $X^{(0)} \equiv -\mu_\ell^{-1}\left[\mathrm{i}H_0, Y^{(0)}\right]$ and

$$Z \equiv 2^{-1}\left[X^{(0)}, Y^{(0)}\right] = \sum_{m=1}^{\ell} \left(\tilde{\delta}_{m-1}^2 - \tilde{\delta}_m^2\right) h_m.$$

Suppose $\mathcal{M} - \{\ell\}$ has ℓ' elements labelled m_1, m_2 up to $m_{\ell'}$ and let $m_{\ell'+1} = \ell$. Then

$$Y^{(1)} \equiv \left[Z, X^{(0)}\right] - v_{m_1} Y^{(0)} = \sum_{k=2}^{\ell'+1} \tilde{\delta}_{m_k}\left(v_{m_k} - v_{m_1}\right) y_{m_k}$$

$$X^{(1)} \equiv \left[Y^{(0)}, Z\right] - v_{m_1} X^{(0)} = \sum_{k=2}^{\ell'+1} \tilde{\delta}_{m_k}\left(v_{m_k} - v_{m_1}\right) x_{m_k}$$

$$Y^{(2)} \equiv \left[Z, X^{(1)}\right] - v_{m_2} Y^{(1)} = \sum_{k=3}^{\ell'+1} \tilde{\delta}_{m_k}\left(v_{m_k} - v_{m_1}\right)\left(v_{m_k} - v_{m_2}\right) y_{m_k}$$

$$X^{(2)} \equiv \left[Y^{(1)}, Z\right] - v_{m_2} X^{(1)} = \sum_{k=3}^{\ell'+1} \tilde{\delta}_{m_k} \left(v_{m_k} - v_{m_1}\right) \left(v_{m_k} - v_{m_2}\right) x_{m_k}$$

$$\vdots$$

$$Y^{(\ell')} \equiv \prod_{k=1}^{\ell'} \tilde{\delta}_\ell \left(v_\ell - v_{m_k}\right) y_\ell$$

shows that $y_\ell \in \mathcal{L}'$ and hence $\mathcal{L}' = sp(\ell)$ by lemma 2 of appendix C. □

A similar argument shows that if there exists $k \in M$ such that $v_m \neq v_k$ for $m, k \in \mathcal{M}$ but $m \neq k$, then $y_k \in \mathcal{L}'$. Using the fact that the generators y_m of $sp(\ell)$ are not diagonal with respect to the Cartan elements (see appendix C), it generally follows that $\mathcal{L}'$ contains all the generators x_m and y_m and thus $\mathcal{L}' = sp(\ell)$ as well. An important special case of this type is a system with $N = 2\ell$ equally spaced energy levels and uniform transition dipole moments.

Theorem 7. *The dynamical Lie algebra $\mathcal{L}'$ generated by a system $H = H_0' + f(t)H_1$ with $N = 2\ell$ equally spaced energy levels and uniform dipole moments is $sp(\ell)$.*

Proof. We have $x_\ell = \omega^{-1}[\mathrm{i}H_0', \mathrm{i}H_1]$, $y_\ell = -2^{-1}[\mathrm{i}H_0', x_\ell]$ and $h_\ell = -2^{-1}[x_\ell, y_\ell]$. Next, set $Y^{(k)} = Y^{(k-1)} - y_{\ell+1-k}$ and $Z^{(k)} = Z^{(k-1)} - h_{\ell+1-k}$ for $1 \leqslant k < \ell$, with $Y^{(0)} = \delta^{-1}\mathrm{i}H_1$ and $Z^{(0)} = \mathrm{i}H_0'$, and note that $x_{\ell-k} = \left[Z^{(k)}, Y^{(k)}\right]$, $y_{\ell-k} = -2^{-1}\left[Z^{(k)}, x_{\ell-k}\right]$ and $h_{\ell-k} = -2^{-1}[x_{\ell-k}, y_{\ell-k}]$. This shows that $\mathcal{L}'$ contains all the generators x_m, y_m of $sp(\ell)$. Hence, $\mathcal{L}' = sp(\ell)$. □

4.3. Application of the criteria

Let us now return to the original system (12). Since we have assumed that the energy levels E_m of the system are ordered in a non-decreasing sequence, i.e., $E_m \leqslant E_{m+1}$ for all m, we have $\mu_m \geqslant 0$, and hence

$$\tilde{E}_m = -\left(\frac{\mu_\ell}{2} + \sum_{s=m}^{\ell-1} \mu_s\right) \leqslant 0 \qquad \tilde{E}_m \leqslant \tilde{E}_{m+1} \qquad 1 \leqslant m \leqslant \ell$$

i.e., the energy levels $\tilde{E}_m$ are negative and form an increasing sequence. Noting that $\tilde{E}_m = \epsilon_m$ we thus have $\omega_m = \epsilon_{m+1} - \epsilon_m = \mu_m \geqslant 0$ for $1 \leqslant m \leqslant \ell - 1$ and $\omega_\ell = 2\epsilon_\ell = \mu_\ell$.

Thus, if $\mu_\ell \neq 0$ and $\mu_m \neq \mu_\ell$ for $m < \ell$ then $\mathcal{L}' = sp(\ell)$ according to theorem 5, independent of the choice of the dipole moments, provided that they are non-zero. If $\mu_m = \mu_\ell$ for some $m < \ell$ then theorem 6 applies and the dipole moments determine whether we have $\mathcal{L}' = sp(\ell)$ or a proper subalgebra.

In particular, the Lie algebra is $sp(\ell)$ if the energy levels are equally spaced, $\mu_m = \mu_\ell$ for all m, and the dipole moments $d_m \neq 0$, $1 \leqslant m \leqslant \ell$, are such that there exists k, $1 \leqslant k \leqslant \ell$, so that $v_m \neq v_k$ for all $m \neq k$, where

$$v_m = 2\tilde{d}_m^2 - \tilde{d}_{m-1}^2 - \tilde{d}_{m+1}^2 = 2d_m^2 - d_{m-1}^2 - d_{m+1}^2 \qquad 1 \leqslant m < \ell$$

(with $d_0 = 0$) and $v_\ell = 2\tilde{d}_\ell^2 - 2\tilde{d}_{\ell-1}^2$.

For instance, setting $d_m = \sqrt{m}$ for $1 \leqslant m \leqslant \ell$ works since it gives $v_m = 2m - (m-1) - (m+1) = 0$ for $1 \leqslant m < \ell$ but $v_\ell = 2$. Similarly, setting $d_m = 1$ for $1 \leqslant m \leqslant \ell$ also gives $\mathcal{L}' = sp(\ell)$ due to theorem 7.

However, recall that there are systems of type (12) whose Lie algebra $\mathcal{L}'$ is a proper subalgebra of $sp(\ell)$, as example 2 above clearly shows. Note that in this example, the energy levels are equally spaced and the dipole moments d_m are such that $v_1 = 2d_1^2 - d_2^2 = 2\times 5 - 8 = 2$, $v_2 = 2d_2^2 - d_1^2 - d_3^2 = 2\times 8 - 5 - 9 = 2$ and $v_3 = 2d_3^2 - 2d_2^2 = 2(9-8) = 2$, i.e., all the v_m are equal and none of the theorems above are applicable.

5. Conclusion

Our analysis of finite-dimensional, non-decomposable driven quantum systems with nearest neighbour interactions and non-zero dipole moments shows that the dynamical Lie algebra $\mathcal{L}'$ generated by the trace-zero part of the internal Hamiltonian and the interaction Hamiltonian of the system is either $su(N)$, $so(N)$, $sp\left(\frac{1}{2}N\right)$, or a simple subalgebra of these. Although by far the most common case is $su(N)$, which corresponds to density matrix/observable controllability and usually complete controllability [3], certain symmetries of the controlled transitions can destroy or reduce the controllability of the system.

Precisely, we showed that the dynamical Lie algebra $\mathcal{L}'$ of a system with symmetrically coupled transitions is a subalgebra of $so(2\ell+1)$ if the system has an odd number of energy levels (where degenerate levels are to be counted according to multiplicity) and a subalgebra of $sp(\ell)$ if the system has an even number of energy levels. Moreover, we established criteria which guarantee in most cases that the dynamical Lie algebra is actually isomorphic to either $so(2\ell+1)$ or $sp(\ell)$. In particular, the dynamical Lie algebra of a system with equally spaced energy levels and uniform transition dipole moments is $so(N)$ if $N = 2\ell+1$, and $sp\left(\frac{1}{2}N\right)$ if $N = 2\ell$.

Despite the rather technical nature of the results presented in this paper, we would like to emphasize that the identification of the dynamical Lie algebra is a crucial first step towards identification of reachable and non-reachable target states for systems that are not essentially controllable. Furthermore, knowledge about the structure of the dynamical Lie algebra can be used to develop efficient control schemes for these systems.

Appendix A. The Lie algebra $su(N)$

A standard basis representation for the Lie algebra $su(N)$ in terms of trace-zero, skew-Hermitian $N\times N$ matrices is (see, for example, [10])

$$x_{m,n} \equiv e_{m,n} - e_{n,m} \qquad y_{m,n} \equiv \mathrm{i}(e_{m,n} + e_{n,m}) \qquad h_m \equiv \mathrm{i}(e_{m,m} - e_{m+1,m+1}) \tag{A.1}$$

where $1 \leqslant m \leqslant N-1$, $m < n \leqslant N$ and $\mathrm{i} = \sqrt{-1}$. There are $\ell = N-1$ generators h_m and $\frac{1}{2}\ell(\ell+1)$ generators of type $x_{m,n}$ and $y_{m,n}$ each. Hence, the total number of generators is N^2-1 and thus the dimension of the Lie algebra $su(N)$ is N^2-1. A nice discussion of controllability of N-level quantum systems in terms of root space decompositions of $su(N)$ can be found in [9].

Appendix B. The Lie algebra $so(2\ell+1)$

$so(N)$ usually refers to the real Lie algebra of trace-zero, anti-symmetric matrices [10]. However, since we are dealing with subalgebras of $su(N)$ generated by $N\times N$ skew-Hermitian matrices, we require a representation of $so(N)$ in terms of trace-zero, skew-Hermitian matrices. For $N = 2\ell+1$, the standard representation of the complex Lie algebra B_ℓ [11] leads to the following skew-Hermitian basis for the real Lie algebra $so(2\ell+1)$:

$$\begin{aligned} h_m &= \mathrm{i}(e_{m+1,m+1} - e_{m+\ell+1,m+\ell+1}) & x_{\epsilon_m} &= x_{1,m+1} - x_{m+\ell+1,1} \\ y_{\epsilon_m} &= y_{1,m+1} - y_{m+\ell+1,1} & x_{\epsilon_m+\epsilon_n} &= x_{m+\ell+1,n+1} - x_{n+\ell+1,m+1} \\ y_{\epsilon_m+\epsilon_n} &= y_{m+\ell+1,n+1} - y_{n+\ell+1,m+1} & x_{\epsilon_m-\epsilon_n} &= x_{n+1,m+1} - x_{m+\ell+1,n+\ell+1} \\ y_{\epsilon_m-\epsilon_n} &= y_{n+1,m+1} - y_{m+\ell+1,n+\ell+1} \end{aligned} \tag{B.1}$$

where $1 \leqslant m \leqslant \ell$ and $m < n \leqslant \ell$. Since there are ℓ elements h_m, x_{ϵ_m} and y_{ϵ_m} each, as well as $\frac{1}{2}\ell(\ell-1)$ elements $x_{\epsilon_m+\epsilon_n}$, $y_{\epsilon_m+\epsilon_n}$, $x_{\epsilon_m-\epsilon_n}$ and $y_{\epsilon_m-\epsilon_n}$ each, the total number of basis elements is $\ell(2\ell+1)$. Thus, the dimension of $so(2\ell+1)$ is $\ell(2\ell+1)$. Using the general commutation relations

$$\begin{aligned} [x_{\epsilon_m}, x_{\epsilon_m-\epsilon_n}] &= x_{\epsilon_n} & [x_{\epsilon_m}, y_{\epsilon_m-\epsilon_n}] &= y_{\epsilon_n} \\ [x_{\epsilon_m}, x_{\epsilon_n}] &= x_{\epsilon_m-\epsilon_n} - x_{\epsilon_m+\epsilon_n} & [x_{\epsilon_m}, y_{\epsilon_n}] &= y_{\epsilon_m-\epsilon_n} + y_{\epsilon_m+\epsilon_n} \\ [x_{\epsilon_m}, y_{\epsilon_m}] &= -2h_m & [x_{\epsilon_m\pm\epsilon_n}, y_{\epsilon_m\pm\epsilon_n}] &= -2(h_m \pm h_n) \\ [h_m, x_{\epsilon_m\pm\epsilon_n}] &= -y_{\epsilon_m\pm\epsilon_n} & [h_m, y_{\epsilon_m\pm\epsilon_n}] &= x_{\epsilon_m\pm\epsilon_n} \end{aligned} \tag{B.2}$$

for $m \neq n$, shows that the elements x_m and y_m with

$$\begin{aligned} x_1 &= x_{\epsilon_1} & x_{m+1} &= x_{\epsilon_m-\epsilon_{m+1}} & 1 &\leqslant m \leqslant \ell-1 \\ y_1 &= y_{\epsilon_1} & y_{m+1} &= y_{\epsilon_m-\epsilon_{m+1}} & 1 &\leqslant m \leqslant \ell-1 \end{aligned} \tag{B.3}$$

are not diagonal with respect to the Cartan elements h_m of the Lie algebra and generate the full Lie algebra $so(2\ell+1)$. Furthermore, it generally suffices to prove that the Lie algebra $\mathcal{L}'$ generated by $\mathrm{i}H_0'$ and $\mathrm{i}H_1$ as in (10) contains one of these elements to conclude that $\mathcal{L}' = so(2\ell+1)$. We shall demonstrate this explicitly for the case $y_1 \in L'$.

Lemma 1. *Let $\mathcal{L}'$ be the Lie algebra generated by $\mathrm{i}H_0'$ and $\mathrm{i}H_1$ as defined in (10). If $y_1 \in \mathcal{L}'$ then $x_m, y_m \in \mathcal{L}'$ for $1 \leqslant m \leqslant \ell$ and hence $\mathcal{L}' = so(2\ell+1)$.*

Proof. Using (B.2) shows that $y_1 \in \mathcal{L}'$ implies $[\mathrm{i}H_0, y_1] = \epsilon_1 x_1$ and $[x_1, y_1] = 2h_1$; thus $x_1, h_1 \in \mathcal{L}'$. Furthermore, we have

$$Z^{(1)} = \mathrm{i}H_0 - \epsilon_1 h_1 = \sum_{m=2}^{\ell} \epsilon_m h_m \qquad Y^{(1)} = \mathrm{i}H_1 - \delta_1 y_1 = \sum_{m=2}^{\ell} \delta_m y_m$$

$$X^{(1)} = -[\mathrm{i}H_0, \mathrm{i}H_1] + \epsilon_1\delta_1 x_1 = \sum_{m=2}^{\ell} (\epsilon_m - \epsilon_{m-1})\delta_m x_m$$

$$\left[Z^{(1)}, Y^{(1)}\right] = -\epsilon_2\delta_2 x_2 - \sum_{m=3}^{\ell} (\epsilon_m - \epsilon_{m-1})\delta_m x_m$$

which shows that $X^{(1)} + \left[Z^{(1)}, Y^{(1)}\right] = -\epsilon_1\delta_2 x_2$, i.e., $x_2 \in \mathcal{L}'$, and $\left[Z^{(1)}, x_2\right] = \epsilon_2 y_2$, $[x_2, y_2] = 2(h_2 - h_1)$ implies $y_2, h_2 \in \mathcal{L}'$. In general, defining recursively

$$Z^{(k)} = Z^{(k-1)} - \epsilon_k h_k \qquad Y^{(k)} = Y^{(k-1)} - \delta_k y_k \qquad X^{(k)} = X^{(k-1)} - (\epsilon_k - \epsilon_{k-1})\delta_k x_k$$

shows that $X^{(k)} + \left[Z^{(k)}, Y^{(k)}\right] = -\epsilon_k\delta_{k+1}x_{k+1}$, $\left[Z^{(k)}, x_{k+1}\right] = \epsilon_{k+1}y_{k+1}$ and $[x_{k+1}, y_{k+1}] = 2(h_{k+1} - h_k)$. Thus, x_{k+1}, y_{k+1} and h_{k+1} are in $\mathcal{L}'$ for $k = 2, 3, \ldots, \ell-1$. □

Appendix C. The Lie algebra $sp(\ell)$

A basis representation for the Lie algebra $sp(\ell)$ for $N = 2\ell$ in terms of trace-zero, skew-Hermitian $N \times N$ matrices can be derived from the standard basis for C_ℓ [11]:

$$\begin{aligned} &h_m = \mathrm{i}(e_{m,m} - e_{m+\ell,m+\ell}) && x_{2\epsilon_m} = x_{m+\ell,m} && y_{2\epsilon_m} = y_{m+\ell,m} \\ &x_{\epsilon_m+\epsilon_n} = x_{m+\ell,n} + x_{n+\ell,m} && y_{\epsilon_m+\epsilon_n} = y_{m+\ell,n} + y_{n+\ell,m} \\ &x_{\epsilon_m-\epsilon_n} = x_{n,m} - x_{m+\ell,n+\ell} && y_{\epsilon_m-\epsilon_n} = y_{n,m} - y_{m+\ell,n+\ell} \end{aligned} \tag{C.1}$$

where $1 \leqslant m \leqslant \ell$ and $m < n \leqslant \ell$. Since there are ℓ elements h_m, $x_{2\epsilon_m}$ and $y_{2\epsilon_m}$ each, as well as $\frac{1}{2}\ell(\ell-1)$ elements $x_{\epsilon_m+\epsilon_n}$, $y_{\epsilon_m+\epsilon_n}$, $x_{\epsilon_m-\epsilon_n}$ and $y_{\epsilon_m-\epsilon_n}$ each, the total number of basis elements is $\ell(2\ell+1)$ and the dimension of $sp(\ell)$ is thus $\ell(2\ell+1)$. Using the general commutation relations

$$\begin{aligned} &[x_{2\epsilon_n}, x_{\epsilon_m-\epsilon_n}] = x_{\epsilon_m+\epsilon_n} && [x_{2\epsilon_n}, y_{\epsilon_m-\epsilon_n}] = y_{\epsilon_m+\epsilon_n} \\ &[x_{\epsilon_m+\epsilon_n}, x_{\epsilon_m-\epsilon_n}] = 2(x_{2\epsilon_m} - x_{2\epsilon_n}) && [x_{\epsilon_m+\epsilon_n}, y_{\epsilon_m-\epsilon_n}] = 2(y_{2\epsilon_m} + y_{2\epsilon_n}) \\ &[x_{2\epsilon_m}, y_{2\epsilon_m}] = -2h_m && [x_{\epsilon_m\pm\epsilon_n}, y_{\epsilon_m\pm\epsilon_n}] = -2(h_m \pm h_n) \\ &[h_m, x_{\epsilon_m\pm\epsilon_n}] = -y_{\epsilon_m\pm\epsilon_n} && [h_m, y_{\epsilon_m\pm\epsilon_n}] = x_{\epsilon_m\pm\epsilon_n} \end{aligned} \tag{C.2}$$

for $m \neq n$, shows that the elements x_m and y_m with

$$\begin{aligned} &x_m = x_{\epsilon_m-\epsilon_{m+1}} && 1 \leqslant m \leqslant \ell-1 && x_\ell = x_{2\epsilon_\ell} \\ &y_m = y_{\epsilon_m-\epsilon_{m+1}} && 1 \leqslant m \leqslant \ell-1 && y_\ell = y_{2\epsilon_\ell}. \end{aligned} \tag{C.3}$$

are not diagonal with respect to the Cartan elements h_m of the Lie algebra and generate the full Lie algebra $sp(\ell)$. Again, it therefore generally suffices to prove that the Lie algebra $\mathcal{L}'$ generated by $\mathrm{i}H_0'$ and $\mathrm{i}H_1$ as in (15) contains one of these elements to conclude that $\mathcal{L}' = sp(\ell)$. We demonstrate this explicitly for the case $y_\ell \in L'$.

Lemma 2. *Let $\mathcal{L}'$ be the Lie algebra generated by $\mathrm{i}H_0'$ and $\mathrm{i}H_1$ defined in (15). If $y_\ell \in \mathcal{L}'$ then $x_m, y_m \in \mathcal{L}'$ for $1 \leqslant m \leqslant \ell$, hence $\mathcal{L}' = sp(\ell)$.*

Proof. Using (C.2) shows that $y_\ell \in \mathcal{L}'$ implies $[\mathrm{i}H_0', y_\ell] = 2\epsilon_\ell x_\ell$ and $[x_\ell, y_\ell] = 2h_\ell$; thus $x_\ell, h_\ell \in \mathcal{L}'$. Furthermore, we have

$$Z^{(1)} = \mathrm{i}H_0' - \epsilon_\ell h_\ell = \sum_{m=1}^{\ell-1} \epsilon_m h_m$$

$$Y^{(1)} = \mathrm{i}H_1 - \delta_\ell y_\ell = \sum_{m=1}^{\ell-1} \delta_m y_m$$

$$X^{(1)} = -[\mathrm{i}H_0', \mathrm{i}H_1] + 2\epsilon_\ell\delta_\ell x_\ell = \sum_{m=1}^{\ell-1} (\epsilon_{m+1} - \epsilon_m)\delta_m x_m$$

$$[Z^{(1)}, Y^{(1)}] = \epsilon_{\ell-1}\delta_{\ell-1}x_{\ell-1} - \sum_{m=1}^{\ell-2} (\epsilon_{m+1} - \epsilon_m)\delta_m x_m$$

which shows that $X^{(1)} + [Z^{(1)}, Y^{(1)}] = \epsilon_\ell\delta_{\ell-1}x_{\ell-1}$, $[Z^{(1)}, x_{\ell-1}] = -\epsilon_{\ell-1}y_{\ell-1}$, and $[x_{\ell-1}, y_{\ell-1}] = 2(h_\ell - h_{\ell-1})$; thus $x_{\ell-1}, y_{\ell-1}, h_{\ell-1} \in \mathcal{L}'$. In general, defining recursively

$$\begin{aligned} &Z^{(k+1)} = Z^{(k)} - \epsilon_{\ell-k}h_{\ell-k} && Y^{(k+1)} = Y^{(k)} - \delta_{\ell-k}y_{\ell-k} \\ &X^{(k+1)} = X^{(k)} - (\epsilon_{\ell-k+1} - \epsilon_{\ell-k})\delta_{\ell-k}x_{\ell-k} \end{aligned}$$

shows that $X^{(k+1)} + [Z^{(k+1)}, Y^{(k+1)}] = \epsilon_{\ell-k}\delta_{\ell-k-1}x_{\ell-k-1}$, $[Z^{(k+1)}, x_{\ell-k-1}] = -\epsilon_{\ell-k-1}y_{\ell-k-1}$ and $[x_{\ell-k-1}, y_{\ell-k-1}] = 2(h_{\ell-k} - h_{\ell-k-1})$. Thus, we have indeed $x_{\ell-k-1}$, $y_{\ell-k-1}$ and $h_{\ell-k-1}$ in $\mathcal{L}'$ for $k = 1, 2, \ldots, \ell-2$. □

Appendix D. The Lie algebra $so(2\ell)$

Using the standard representation for the complex Lie algebra D_ℓ [11], we can derive the following skew-Hermitian basis for $so(2\ell)$:

$$\begin{aligned} &h_m = \mathrm{i}(e_{m,m} - e_{m+\ell,m+\ell}) && x_{\epsilon_m+\epsilon_n} = x_{m+\ell,n} - x_{n+\ell,m} \\ &y_{\epsilon_m+\epsilon_n} = y_{m+\ell,n} - y_{n+\ell,m} && x_{\epsilon_m-\epsilon_n} = x_{n,m} - x_{m+\ell,n+\ell} \\ &y_{\epsilon_m-\epsilon_n} = y_{n,m} - y_{m+\ell,n+\ell} \end{aligned} \tag{D.1}$$

where $1 \leqslant m \leqslant \ell$ and $m < n \leqslant \ell$. There are ℓ elements h_m, as well as $\frac{1}{2}\ell(\ell-1)$ elements $x_{\epsilon_m+\epsilon_n}$, $y_{\epsilon_m+\epsilon_n}$, $x_{\epsilon_m-\epsilon_n}$ and $y_{\epsilon_m-\epsilon_n}$ each, i.e., the total number of basis elements is $\ell(2\ell-1)$. Thus, the dimension of $so(2\ell)$ is $\ell(2\ell-1)$.

To see why there is no (2ℓ)-level system with $H = H_0 + f(t)H_1$, where $\mathrm{i}\hat{H}_0$ and $\mathrm{i}\hat{H}_1$ are as defined in (2) and (5), respectively, such that $\mathcal{L}' = so(2\ell)$, note that

$$\begin{aligned} &x_m = x_{\epsilon_m-\epsilon_{m+1}} && 1 \leqslant m \leqslant \ell-1 && x_\ell = x_{\epsilon_{\ell-1}+\epsilon_\ell} \\ &y_m = y_{\epsilon_m-\epsilon_{m+1}} && 1 \leqslant m \leqslant \ell-1 && y_\ell = y_{\epsilon_{\ell-1}+\epsilon_\ell}. \end{aligned} \tag{D.2}$$

forms a minimal, complete set of generators for $so(2\ell)$ if $\ell \geqslant 2$. Each of the ℓ generators y_m has four distinct, non-zero entries, which corresponds to a total of 4ℓ non-zero entries. However, $\mathrm{i}H_1$ for a (2ℓ)-level system with only nearest neighbour interactions can have at most $2(2\ell-1) = 4\ell-2$ non-zero entries on the first super- and sub-diagonal. Hence, a (2ℓ)-level system with dynamical Lie algebra $so(2\ell)$ must have interactions between non-adjacent energy levels.

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