Corrections, Additions and Comments to the Book: 'Introduction to Quantum Control and Dynamics'

Domenico D'Alessandro*

July 29, 2008

This document contains several corrections, additions, improvements and comments to my book 'Introduction to Quantum Control and Dynamics'. It will be periodically updated. Most of the corrections concern minor typos but others are more substantial and require a better specification of some hypothesis, mathematical procedure or results. Since the publication of the book I have found several points where the presentation could be more clear and complete. Moreover I have received and I always appreciate constructive criticism and suggestions from friends and colleagues. In providing this document I hope to render the book more readable and useful.

Chapter 1

subsection 1.1.1.2

It should be mentioned here that the Dirac notation is also useful to denote the eigenvector corresponding to a given eigenvalue, in that the eigenvector corresponding to the eigenvalue λ is denoted by $|\lambda\rangle$.

subsection 1.1.5.2

It should be pointed out here that what is called here 'matrix vector representation' is nothing but what is called 'coordinatization' in elementary linear algebra, the process which reduces every finite dimensional vector space to $\mathbb{C}^n$.

subsection 1.2.1.1

On page 18, line 7

$\lim_{\epsilon \to 0} P_{\lambda+\epsilon} = P_\lambda$ should be $\lim_{\epsilon \to 0^+} P_{\lambda+\epsilon} = P_\lambda$

subsection 1.3.1.2

*Department of Mathematics, Iowa State University, Ames, Iowa, U.S.A. Electronic address: daless@iastate.edu

When mentioning *canonical quantization* on page 27 it should be said that canonical quantization is treated in Chapter 2, section 2.1.2.

subsection 1.3.1.3

Liouville's equation is also called **Von Neumann equation**

subsection 1.4.2

The reasoning could be extended to any pair of nondegenerate observables one on subsystem 1 and the other concerning subsystem 2. The number of possible results of the combined measurement of these observables is $n_1 n_2$ and to each result there corresponds an eigenvector in an orthogonal basis.

subsection 1.5

Add an exercise: in the same situation as Exercise 1.4 show that the matrix representation of a tensor product of two operators A and B is the Kronecker product of the matrix representation of A and the matrix representation of B.

Chapter 2

In introduction to the chapter. Replace
'to derive the models' with 'to derive the appropriate models'
'as bilinear systems' with 'of bilinear systems'
'evolution is determined by an element of the Lie group' with 'evolution is a curve in the Lie group'

subsection 2.1.2.2

In the title, replace
'variables concerning' with 'variables describing'

subsection 2.1.3

pg. 52, Replace Scrhödinger with Schrödinger

Chapter 3

subsection 3.1.1.1

It should be said that 'Unless otherwise specified the Lie algebras considered in the following are intended to be over the field of reals'.

subsection 3.1.2.3

pg. 81, Replace 'one can prove if' with 'one can prove that if'

The correspondence in the FACT is often called *Lie correspondence* (cf., e.g, Section 2.5., [5]).

section 3.2

Theorem 3.2.1 As it is stated Theorem 3.2.1 (and its proof) tacitly assumes that $e^{\mathcal{L}}$ is in fact a Lie subgroup of $U(n)$ in the sense of Definition 3.1.7. In particular, $e^{\mathcal{L}}$ is a Lie group with the topology induced by the one of $U(n)$. The proof presented in Appendix D in the last part (end of page 312 beginning of page 313) uses this assumption. Without this assumption, one can still define the Lie group $e^{\mathcal{L}}$ but it is not true that $\mathcal{R} = e^{\mathcal{L}}$. For example, if Schrödinger operator equation is $\dot{X} = -iH_0X$, with

$$H_0 = \begin{pmatrix} 0 & i & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & ix \\ 0 & 0 & -ix & 0 \end{pmatrix},$$

with x an irrational number, $\mathcal{R} = \{e^{-iH_0t} | t \geq 0\}$ while $e^{\mathcal{L}} = \{e^{-iH_0t} | t \in \mathbf{R}\}$ and the two sets do not coincide.[1]

The first two parts of the proof presented in Appendix D ('$\mathcal{R}$ is dense in $e^{\mathcal{L}}$' and 'Finite generation of $e^{\mathcal{L}}$') remain however true without this assumption. In particular we can always drive the evolution operator to a value arbitrarily close to any value in $e^{\mathcal{L}}$ (in the topology induced by the one of $U(n)$). Therefore, from a practical point of view $\mathcal{R}$ is almost the same as $e^{\mathcal{L}}$, and it is exactly the same when $e^{\mathcal{L}}$ is a Lie subgroup of $U(n)$.

It is interesting to study when $e^{\mathcal{L}}$ is a Lie subgroup of $U(n)$. This is a classical question in Lie theory which is often referred to as the correspondence between Lie subgroups and Lie subalgebras. A classical result which is known as the **closed subgroup theorem** (cf., e.g., [5] Corollary 3 of §2.7 and Exercise 2, therein) tells us that $e^{\mathcal{L}}$ is a Lie subgroup if and only if it is closed in the topology of $U(n)$. From a practical point of view, it is of interest to have a way to check this property on the Lie algebra $\mathcal{L}$. The Killing form whose definition is given in Appendix C, Section C.1, gives a way to check this: We have (see, e.g., Proposition 4.27 in [3])

Theorem *If the Killing form of $\mathcal{L}$ is negative definite, then $e^{\mathcal{L}}$ is a compact Lie group (and therefore is closed).*

This is an important result which allows us to check a topological property using an algebraic test. However it only gives a sufficient condition and does not use further structure of $\mathcal{L}$. A better alternative in my opinion is to notice that the dynamical Lie algebra $\mathcal{L}$, being a subalgebra of $u(n)$ is always of the form

$$\mathcal{L} = [\mathcal{L}, \mathcal{L}] \oplus \mathcal{Z} \tag{1}$$

where $[\mathcal{L}, \mathcal{L}]$ is a semisimple Lie algebra and $\mathcal{Z}$ is the center of $\mathcal{L}$, i.e., the subspace of all the matrices that commute with all of $\mathcal{L}$, which is an Abelian subalgebra of $\mathcal{L}$.

[1] I thank Francesco Ticozzi for pointing out this example to me.

Moreover $[\mathcal{L}, \mathcal{L}]$ and $\mathcal{Z}$ commute. The decomposition (1) can always be computed with linear algebra calculations.

As a consequence of the decomposition (1) $e^{\mathcal{L}}$ is always the product of a the Lie group $e^{[\mathcal{L},\mathcal{L}]}$ with the Abelian Lie group $e^{\mathcal{Z}}$, i.e., every $X \in e^{\mathcal{L}}$ can be written as $X = PZ = ZP$ with $P \in e^{[\mathcal{L},\mathcal{L}]}$ and $Z \in e^{\mathcal{Z}}$. At this point, using the fact that $e^{[\mathcal{L},\mathcal{L}]}$ is a semisimple Lie group and a subgroup of a compact Lie group ($U(n)$) we can apply Theorem 6.3.13 of [4] which says:[2]

Theorem *If $\mathcal{G}$ is a semisimple Lie subalgebra of a Lie algebra $\mathcal{H}$ and $e^{\mathcal{H}}$ is a compact Lie group (such as $U(n)$) then $e^{\mathcal{G}}$ is a Lie subgroup of $e^{\mathcal{H}}$.*

Therefore problems may only come from the Abelian part $\mathcal{Z}$ which has usually small dimension and it is easy to analyze. $e^{\mathcal{Z}}$ is the same as $T^k \times \mathbf{R}^j$ where T^k is a k-torus (which is compact). The Lie group $e^{\mathcal{L}}$ is compact if $j = 0$. Further discussion on the decomposition (1) can be found in my recent paper [1]. This method of decompositions of the Lie group allows not only to check whether $e^{\mathcal{L}}$ is closed or not but also to check where, possibly, the non-closedness comes from.

Another linear algebra type of test is suggested in Problem 4 of §2.7. of [5]. If for $X \in u(n)$, $[X, \mathcal{L}] \subseteq \mathcal{L}$ implies $X \in \mathcal{L}$, then $e^{\mathcal{L}}$ is a closed subgroup.

Remark (*To a certain extent, the proof of controllability is constructive*) Assume we wish to drive the evolution operator X from the identity to $X_f \in e^{\mathcal{L}}$. Assume $e^{\mathcal{L}}$ is closed and therefore compact, as discussed above.[3] In this case, the exponential map is onto (cf. Corollary 4.48 in [3]), that is, there exists a matrix $A \in \mathcal{L}$ such that $e^A = X_f$, for every X_f. This also means that given any neighborhood N of the identity in $e^{\mathcal{L}}$, we can choose n sufficiently large such that $e^{\frac{A}{n}} = X_f^{\frac{1}{n}} \in N$. Now, assume first that we have available in the set $\text{span}_{u \in \mathcal{U}}\{-iH(u)\}$ a basis of elements (Hamiltonians) for $\mathcal{L}$. That is, no Lie bracket is necessary to obtain a basis of $\mathcal{L}$. Let $m := \dim \mathcal{L}$. There exist m values of the control u_j, and corresponding m matrices $A_j := -iH(u_j)$, $j = 1, \ldots, m$, (cf. Lemma 1 in Appendix D) which form a basis for $\mathcal{L}$. By varying $t_1, \ldots, t_m$ in a neighborhood of the origin in $\mathbf{R}^m$, $e^{A_m t_m} e^{A_{m-1} t_{m-1}} \cdots e^{A_1 t_1}$ gives a neighborhood of the identity in $e^{\mathcal{L}}$ and in particular it contains $e^{\frac{A}{n}}$. Therefore, there exist values $\bar{t}_1, \ldots, \bar{t}_m$ such that setting the control equal to u_1 for time $\bar{t}_1$ and then equal to u_2 for time $\bar{t}_2$, and so on, up to, equal to u_m for time $\bar{t}_m$, we drive the value of the evolution operator to $e^{\frac{A}{n}}$. Obviously this argument ignores the fact that some of the values $\bar{t}_j$, $j = 1, ..., m$, may be negative. However, this is not a big problem. In fact, in many quantum mechanical models, it is possible to choose the controls u_j and therefore the matrices A_j so that the orbits $\{e^{A_j t} | t \in \mathbf{R}\}$ are periodic, which allows us to assume all the $\bar{t}_j$'s positive, without loss of

[2] Notice that the definition of Lie subgroup in [4] is different from the one adopted in my book. However I state the theorem in a form coherent with my notations and definitions.

[3] In the case $e^{\mathcal{L}}$ is not compact the arguments below can be adapted. Instead of writing X_f as $X_f = e^A$ for a certain A, we write X_f as a product of exponentials (as from the correspondence between Lie groups and Lie algebras of pg. 81) and then repeat the arguments below for each exponential. Clearly this presupposes that we are able to write X_f as a product of exponentials.

generality. If this is not the case using the compactness of the Lie group $e^{\mathcal{L}}$, an argument as the one used on pg. 309 of Appendix D (cf. [2]) shows that we can choose a $\tilde{t}_j$ positive such that $e^{\tilde{t}_j A_j}$ is arbitrarily close to $e^{\bar{t}_j A_j}$.

In the more common case where it is not possible to choose controls to obtain a basis of $\mathcal{L}$, we can proceed as in the proof of Lemma 1, Appendix D. Let $\{A_1, \ldots, A_s\}$ be a set of linearly independent available elements (Hamiltonians) which generate $\mathcal{L}$. There exist two values $1 \leq k, l \leq r$ such that the commutator $[A_l, A_k]$ is linearly independent of $\{A_1, \ldots, A_r\}$. This implies that there exists a value $t \in \mathbf{R}$ such that $F := e^{A_l t} A_k e^{-A_l t}$ is also linearly independent, so that we can add F to $\{A_1, \ldots, A_s\}$, to obtain $s+1$ linearly independent matrices in $\mathcal{L}$. Notice that it is very easy to obtain the exponential of F, since $e^{F\tilde{t}} = e^{A_l t} e^{A_k \tilde{t}} e^{-A_l t}$. If the dimension of $\mathcal{L}$ is $s+1$ we have now a basis of $\mathcal{L}$ and we can proceed as above. If this is not the case, we can obtain more linearly independent matrices in the same way and eventually obtain a basis of $\mathcal{L}$. From this basis, using only exponentials of the available elements we obtain all the elements of a neighborhood of the identity in $e^{\mathcal{L}}$ including $e^{\frac{A}{n}}$. Repeating the associated control sequence n times we obtain e^A.

Summarizing, this approach allows us to drive the evolution operator X from the identity to any point in a neighborhood of the identity and therefore to $e^{\frac{A}{n}}$ for n sufficiently large. The main problem with this approach is to find a suitable way to estimate the 'size' of the neighborhood of the identity which is obtained so that so as to know how to choose n so that $e^{\frac{A}{m}}$ is in it. This is an interesting topic for further research.

subsection 3.2.2

Corollary 3.2.3 In Corollary 3.2.3 part b) the topology is the one induced by the one of $U(n)$, which coincides with the one of $e^{\mathcal{L}}$ since we are assuming that $e^{\mathcal{L}}$ is a Lie subgroup of $U(n)$. This corollary could have been stated in a slightly modified form if we did not assume that $e^{\mathcal{L}}$ is a Lie subgroup of $U(n)$. Part a) still holds but with $t_1, \ldots, t_r \geq 0$ replaced by $t_1, \ldots, t_r \in \mathbf{R}^r$ and in part b) the topology is the one of $e^{\mathcal{L}}$.

subsection 3.4.3

After 'determinant equal to one' on page 88 add '(notice that $n \geq 2$)'

subsection 3.4.4

On page 89, modify the sentence '$Sp(k)$ is the group...' as 'By noticing that (3.17) could have been written as $X^T J X = J$, it is easy to see that $Sp(k)$ is the group...'.

subsection 3.6

Theorem 3.6.1 (in the sufficiency proof given in [5] we refer to in the book) also assumes the implicit assumption that $e^{\mathcal{L}}$ is a Lie subgroup of $U(n)$. Therefore the considerations we have explained concerning Theorem 3.2.1 hold in this case, in particular for what concerns the methods to check this assumption. The same word of caution holds in application of **Theorem 3.6.2**, **Corollary 3.6.3** and **Example 3.6.4**. I am not aware of an example of a Lie algebra $\mathcal{L}$ and a density matrix ρ_0 not multiple of the identity such that (3.31) holds and $\mathcal{L}$ is not semi-simple (We have seen above that $\mathcal{L}$ semisimple implies $e^{\mathcal{L}}$ closed) or, more in general, $e^{\mathcal{L}}$ not closed. It is an open question whether such cases exist at all.

subsection 3.7.4

Related to the problem of controllability and the uniform finite generation described in subsection 3.2.2, is the question of computational complexity in quantum computation. One has a collection of Hamiltonians $\{H_j\}$ and wants to know how many gates of the form eH_jt has to put in a cascade to obtain a given unitary which solves a particular computational problem. The question of computational complexity is how this number depends on the size of the data. This is a very big area of research which can take different directions and use different tools. Some results can be found in [155], [125] and [**?**], [**?**].

section 3.8

Add the following exercise

Exercise 3.12: Consider the Lie algebra $\mathcal{L}$ spanned by $\{i\sigma_x \otimes \mathbf{1}, i\sigma_y \otimes \sigma_{x,y,z}, i\sigma_z \otimes \sigma_{x,y,z}, i\mathbf{1} \otimes \sigma_{x,y,z}\}$, where $\sigma_{x,y,z}$ are the Pauli matrices defined in (1.20). Use the test of Theorem 3.6.2 to prove that a system with Lie algebra $\mathcal{L}$ is PSC.

Chapter 4

Chapter 5

Chapter 6

Chapter 7

Chapter 8

Chapter 9

Appendix A

Appendix B

Appendix C

Appendix D

See the discussion above about section 3.2.

Appendix E

Appendix F

References

[1] D. D'Alessandro, Lie Algebraic Analysis and Control of Quantum Dynamics; Applications to quantum walks, xxx.lanl.gov, quant-ph 0803.1193.

[2] M. R. Dowling and M. A. Nielsen, The geometry of quantum computation, xxx.lanl.gov, quant-ph/0701004.

[3] V. Jurdjević and H. Sussmann, Control systems on Lie groups, *Journal of Differential equations*, 12, 313-329, (1972).

[4] A. Knapp, *Lie Groups Beyond an Introduction*, Birkhäuser, Boston, 2-nd ed., 2002.

[5] M. Mottonen and J.J. Vartiainen, Decompositions of general quantum gates, Ch. 7 in Trends in Quantum Computing Research (NOVA Publishers, New York), 2006.

[6] J.F. Price, *Lie Groups and Compact Groups*, London Mathematical Society Lecture Note Series, 25, Cambridge University Press, Cambridge U.K. 1977.

[7] W. Rossmann, *Lie Groups. An Introduction Through Linear Groups*, Oxford Graduate Texts in Methematics-5, Oxford University Press Inc., New York, 2002.