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On the controllability of quantum-mechanical systems

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The systems-theoretic concept of controllability is elaborated for quantum-mechanical systems, sufficient conditions being sought under which the state vector ψ can be guided in time to a chosen point in the Hilbert space $\mathscr{H}$ of the system. The Schrödinger equation for a quantum object influenced by adjustable external fields provides a state-evolution equation which is linear in ψ and linear in the external controls (thus a bilinear control system). For such systems the existence of a dense analytic domain $\mathscr{D}_\omega$ in the sense of Nelson, together with the assumption that the Lie algebra associated with the system dynamics gives rise to a tangent space of constant finite dimension, permits the adaptation of the geometric approach developed for finite-dimensional bilinear and nonlinear control systems. Conditions are derived for global controllability on the intersection of $\mathscr{D}_\omega$ with a suitably defined finite-dimensional submanifold of the unit sphere $S_{\mathscr{H}}$ in $\mathscr{H}$. Several soluble examples are presented to illuminate the general theoretical results.

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I. INTRODUCTION

This paper is devoted to a formal investigation of the controllability of quantum-mechanical systems. Such a study is ultimately motivated by the importance, or potential importance, of precision methods for influencing the dynamical behavior of microsystems, in such diverse contexts as particle acceleration and detection, plasma physics, magnetic resonance, electron microscopy, modern solid-state technology, laser fusion, and optical communication. On the one hand, we may be interested in governing the time development of certain pertinent average quantities. More ambitiously, we may wish to guide the quantum state itself. It is this latter type of controllability which concerns us here.

A. Problem formulation

Consider a physical system whose state $\psi(t)$ evolves with time according to the law

$$\frac{d}{dt}\psi(t) = H_0\psi(t) + \sum_{l=1}^{r} u_l(t) H_l \psi(t), \quad \psi(0) = \psi_o, \quad (1)$$

where ψ is a point in some abstract state space, $H_0, H_1, \ldots, H_r$ are operators in this space, and the $u_l(t)$ are time-dependent scalar control functions. For the case that $H_0, H_1, \ldots, H_r$ are linear operators, we say, in systems-theoretic parlance, that (1) is a *bilinear* system[1] since the last term is simultaneously linear in the state ψ and the controls u_l. The formulation (1) includes as a special case the dynamical law followed by a pure state in quantum theory, i.e., the Schrödinger equation

$$i\hbar \frac{d}{dt}\psi(t) = \left[H_0' + \sum_{l=1}^{r} u_l(t) H_l' \right] \psi(t), \quad (2)$$

where $H_0', H_1', \ldots, H_r'$ are linear, Hermitian operators in the underlying state space $\mathscr{H}$ of the quantum-mechanical system and the u_l are real functions of t. The operator $H_0' \equiv i\hbar H_0$ is naturally interpreted as the Hamiltonian determining the free evolution of the quantum system, while the $u_l H_l' \equiv i\hbar u_l H_l$ represent its couplings or interactions with certain external agents. Through suitable adjustment of the c-number controls $u_l(t)$, these interactions may be used to guide the state $\psi(t) \in \mathscr{H}$.

One may also entertain *linear* control systems, such that none of the controls u_l appears in the same addend with the state ψ, as well as *nonlinear* systems of the form (1) but with one or more of the operators of $\{H_0, H_l\}$ nonlinear. However, these cases are of no immediate relevance to conventional quantum mechanics.

In general, the quantum-mechanical state space $\mathscr{H}$ is an infinite-dimensional Hilbert space. Although the H_l, if not H_0, could in principle depend on t, we shall confine our attention to the case that all these operators are time-independent. We further suppose that the u_l are piecewise-constant functions of t, the intervals of constancy being denoted $[t_i, t_{i+1})$, i integral. Under the stated conditions, the existence and uniqueness of a solution $\psi(t)$ between successive switching times t_i and t_{i+1} is guaranteed by the assumed quantum dynamics. During the prescribed interval, $H_0 + \Sigma_l u_l H_l$ is a constant, skew-Hermitian operator. Patently, there is associated with that operator a unique unitary operator $U(t, t_i)$, parametrized by t on $[t_i, t_{i+1})$, with the property $U(t, t_i)\psi(t_i) = \psi(t)$, where $U(t_i, t_i) = E$ (identity operator). One may therefore proceed to patch together the solutions for the separate intervals to obtain an acceptable, continuous solution $\psi(t)$, over the full range $t \in \mathbb{R}^+$.

Now, a differential system such as (1) is said to be *controllable* if, given two states ψ_o and ψ_f, there exists a time interval $[0, t_f]$ and a set of admissible controls $u_l(t)$ (in our case, piecewise-constant controls), such that the system trajectory beginning at $\psi(0) = \psi_o$ develops under the influence of $u(t)$ to arrive at $\psi(t_f) = \psi_f$. This concept has become one of the touchstones of mathematical systems theory,[2] a discipline deeply rooted in classical dynamics. It is our purpose to introduce the controllability concept into the quantum do-

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main and explore its limitations in that more fundamental setting.

B. Relevant prior work

In recent years substantial progress has been made, based in part on the seminal work of Chow,[3] toward understanding continuous-time finite-dimensional bilinear and (certain) nonlinear systems.[1,4–21] However, the quantum control problem is intrinsically infinite-dimensional. Thus the advances made in Refs. 1 and 4–21 cannot be applied directly to the problem of guiding quantum states—except in idealized situations where the state space becomes finite-dimensional (as when only spin degrees of freedom play a role).

Infinite-dimensional bilinear and nonlinear control systems have not been extensively investigated, although several pioneering efforts deserve note: (i) Both Koch[22] and Brockett[23] have addressed the problem of realization of infinite-dimensional bilinear systems. (ii) Stefan[24] has obtained results on local integrability of a special class of infinite-dimensional control systems. (iii) Ball and Slemrod[25] have established criteria for local stabilization of infinite-dimensional bilinear systems. (iv) Hermes[26,27] has determined sufficient conditions for local controllability of nonlinear delay and infinite-dimensional nonlinear systems.

To the authors' knowledge, very little has been published on the controllability of quantum systems *per se*. As a preliminary to the present work, Tarn, Huang, and Clark[28] have explored the formal basis for the modeling of quantum-mechanical control systems by appropriate Schrödinger equations. Earlier, Butkovskii and Samoilenko[29,30] discussed the control of quantum objects in broad terms and laid out a framework for further studies; a number of enlightening examples were treated, but mathematically definitive results were not presented. Recently, these last workers have announced general conditions for controllability of pure quantum states.[31] However, these findings must be viewed with some caution, since results for finite-dimensional bilinear systems were taken over from Refs. 11 and 12 without due attention to the domain problem for the relevant operators in Hilbert space.

C. Epitome of present approach

In the present contribution, we shall deal with the domain issue for the operators involved in quantum control—which are generally unbounded operators—by appealing to certain fundamental developments due to Nelson.[32,33] That is, we shall pursue our analysis with respect to an analytic domain of the Hilbert space: a dense domain invariant under the action of the given operators, on which the solution $\psi(t)$ of the Schrödinger equation can be expressed globally in exponential form. The existence of such a domain (in some interesting situations) is guaranteed by a theorem of Nelson. Against this underpinning, we are able to extend the geometric approach as implemented by Sussmann and Jurdjevic,[10,11] Krener,[14] Brockett,[16] Kunita,[19] and others (who are concerned only with bounded operators) to establish a series of global controllability conditions for the quantum case. It will be seen both formally and intuitively that, within the assumed framework based on piecewise-constant controls, global controllability on an *infinite*-dimensional submanifold of Hilbert space can never be attained in a practical sense: In general, a desired goal in the state space cannot be achieved with a finite number of manipulations of the control set $\{u_l(t)\}$. Accordingly, our detailed considerations regarding global control are narrowed to situations in which the Lie algebra $\mathscr{A}$ of the operators entering the quantum version of (1) yields a tangent space of constant, finite dimension.

Indeed, if we have to appeal to Nelson's theorem to assure the existence of an analytic domain, then we are already dealing with the following situation. The quantum system is one described by a finite-dimensional Lie group Γ, which is represented by unitary evolution operators on a Hilbert space $\mathscr{H}$. The control system—a bilinear system whose states are in $\mathscr{H}$—has the property that its associated Lie algebra is contained in the Lie algebra of operators on $\mathscr{H}$ obtained from the unitary representation of Γ. This specification is admittedly quite restrictive; therefore, it is not surprising that, with minimal attention to the infinite dimensionality of $\mathscr{H}$, we can bring to bear the techniques introduced for finite-dimensional manifolds in Refs. 10, 11, 14, 16, and 19. One may expect essential differences between finite-dimensional and infinite-dimensional problems to surface as one goes beyond the case of analytic vectors as initial conditions. The next step beyond analytic vectors and toward a less restrictive physical setting might involve "infinitely differentiable vectors"—those vectors of $\mathscr{H}$ for which the orbits are infinitely differentiable functions of the group parameters.

We hasten to point out that the above specification corresponding to Nelson's theorem does include the physical example of paramount importance in engineering applications, namely, the harmonic oscillator with coupling to external classical fields.

D. Organization of the paper

This paper is divided into six main sections. In Sec. II we collect certain key ideas and terminology from manifold theory and Lie algebra which are instrumental to our analysis of the control system (1) in infinite-dimensional space. Section III surveys the existing results on controllability for a finite-dimensional state space. In Sec. IV we introduce the concepts of analytic domain and analytic controllability, consider the implications of Nelson's theorem, and present arguments to the effect that, on an analytic domain, the controllability results obtained for a finite-dimensional state space can be extended to the quantum problem posed in Sec. IA. In Sec. V some examples are given to illustrate the concept of quantum controllability and the general findings of Sec. IV. We conclude, in Sec. VI, with a brief prospectus of outstanding problems in the largely unexplored intersection between quantum mechanics and mathematical systems theory.

II. MATHEMATICAL PRELIMINARIES

In general, the states of a quantum system are represented by vectors (or functions) in an infinite-dimensional space. With this in mind, we shall outline the essential manifold and Lie group theory appropriate to a Banach space. It is assumed that the reader has some familiarity with differentiable manifolds in the finite-dimensional context. In setting up the necessary catalog of concepts, we shall adhere closely to the conventions of Refs. 34–37.

A. Atlases and differentiable manifolds

As in the finite-dimensional case, the concept of *atlas* is introduced as a first step.[35,36] An atlas of a set M is again a collection of *charts* $(\mathsf{U}_i, \varphi_i)$, with $\cup_i \mathsf{U}_i = \mathsf{M}$. But now the bijective map φ_i is from the subset U_i of M onto some open subset of the *Banach space* $\mathscr{E}$, and for every pair i, j the set $\varphi_i(\mathsf{U}_i \cap \mathsf{U}_j)$ is open in $\mathscr{E}$. The atlas is said to be of class C^p if the mapping $\varphi_j \circ \varphi_i^{-1}$: $\varphi_i(\mathsf{U}_i \cap \mathsf{U}_j) \to \varphi_j(\mathsf{U}_i \cap \mathsf{U}_j)$ is of class C^p. (The cases "C^∞" and "analytic" are specified analogously.) For $\mu \in \mathsf{U}_i \subset \mathsf{M}$, the point $\varphi_i(\mu) \in \mathscr{E}$ is the *representative* of μ in the chart $(\mathsf{U}_i, \varphi_i)$.

The next step is to define a C^p *(-differentiable) manifold* modeled on $\mathscr{E}$, as a set M together with an equivalence class of C^p atlases modeled on $\mathscr{E}$. An equivalence relation is provided by the notion of *compatibility*: Two C^p atlases on M are compatible if their union is another such atlas. (To define C^∞-differentiable manifold and analytic manifold, proceed analogously.)

An example may be helpful at this point. Let the set M be $L^2(\mathbb{R}^n)$, let the U_i be open subsets of M with union equal to $L^2(\mathbb{R}^n)$, and let φ_i be the identity mapping. Then clearly M is a C^∞-differentiable and analytic manifold modeled on itself.

B. Tangent vectors, tangent bundles, and vector fields

Equivalent definitions[36] of *tangent vector* to M at point μ may be given (a) in terms of an equivalence class of curves and (b) in terms of the behavior of the representative of the object in question, under a change of charts.

Here we shall give explicit expression only to conception (a).

Definition: A parametrized curve γ on M is a mapping from $\mathsf{J} \subset \mathbb{R}$ into M via $t \in \mathsf{J} \to \gamma(t) \in \mathsf{M}$.

Consider all differentiable curves γ: $\mathsf{J} \subset \mathbb{R} \to \mathsf{M}$ such that $\gamma(0) = \mu \in \mathsf{M}$. We shall regard γ_1 as equivalent to γ_2 if in some chart (U, φ) (consequently,[35,36] in every chart) we have

$$\frac{d}{dt}(\varphi \circ \gamma_1)\bigg|_{t=0} = \frac{d}{dt}(\varphi \circ \gamma_2)\bigg|_{t=0}.$$

Definition: A *tangent vector* at μ to the manifold M, denoted $X\mu$ or $X(\mu)$, is defined by any one such equivalence class. The set of all such equivalence classes constitutes the *tangent-vector space* to M at μ, denoted $\mathscr{T}_\mu(\mathsf{M})$. The vector $v_\mu \equiv d(\varphi \circ \gamma)/dt\,|_{t=0}$ is termed the *representative*, in the chart (U, φ), of the vector tangent at μ to curve γ.

One may establish[35] that $\mathscr{T}_\mu(\mathsf{M})$ is isomorphic to $\mathscr{E}$ and accordingly has an intrinsic vector-space structure.

Definition: The *tangent fiber bundle* T(M) is given by $\cup_{\mu \in \mathsf{M}} \mathscr{T}_\mu(\mathsf{M})$.

It is important to note[35,36] that T(M) has the structure of a differentiable manifold modeled on $\mathscr{E} \times \mathscr{E}$. Further, T(M) has a fiber bundle structure characterized by *base* M, *projection* π:$(\mu, X\mu) \to \mu$, *typical fiber* $\mathscr{E}$, and *structure group* $\mathrm{GL}(\mathscr{E})$.

We are now equipped to formalize the idea of vector field for the case of an infinite-dimensional state space.[36]

Definition: A *vector field* X on a C^p (respectively, C^∞ or analytic) manifold M is a *cross section* of the tangent bundle T(M), by which we mean a class-C^{p-1} (respectively, class-C^∞ or analytic) mapping X: $\mathsf{M} \to \mathsf{T}(\mathsf{M})$, namely, X: $\mu \to (\mu, X\mu)$, such that $\pi \circ X$ is the identity.

C. Submanifolds, tangent subbundles, and integrability

Let M be a C^p manifold, $p \geqslant 0$, and consider a subset $\mathsf{N} \subset \mathsf{M}$ which still has C^p-manifold structure; then N will be called a *submanifold* of M. (The definition of a C^∞ or analytic submanifold runs parallel.) Between N and M there are some natural connections established by mappings (e.g., inclusive mappings). A thorough discussion is contained in Ref. 35. The tangent-vector space of N at μ is a subspace of $\mathscr{T}_\mu(\mathsf{M})$, the latter being, as we recall, an isomorphism of the Banach space $\mathscr{E}$. We can decompose $\mathscr{E}$ into Banach spaces $\mathscr{E}_1$ and $\mathscr{E}_2$ according to $\mathscr{E} = \mathscr{E}_1 \times \mathscr{E}_2$, where $\times$ indicates the Cartesian product and $\mathscr{T}_\mu(\mathsf{N})$ is an isomorphism of $\mathscr{E}_1$. The relationship of N to M can also be framed in terms of the tangent mappings[35,37] $\mathscr{T}_\mu i$: $\mathscr{T}_\mu(\mathsf{N}) \to \mathscr{T}_\mu(\mathsf{M})$ and Ti: $\mathsf{T}(\mathsf{N}) \to \mathsf{T}(\mathsf{M})$ induced by the inclusion i: $\mathsf{N} \to \mathsf{M}$.

Next there arises the notion of tangent subbundle (a subbundle of the tangent bundle over M). For details, see Refs. 35 and 36. A tangent subbundle corresponding to the submanifold N is specified in the same fashion as T(M), with N playing the role of M. But suppose, on the other hand, that we are *given* a tangent subbundle structure $\mathsf{S} \subset \mathsf{T}(\mathsf{M})$, and asked to determine whether or not there exists a submanifold—again call it N—which has tangent bundle S. This is the *integrability problem*. A simplified definition of integrability follows.

Definition: A tangent subbundle S over M is said to be *completely integrable*[38] at a point $\mu_0 \in \mathsf{M}$ if there exists a submanifold N of M containing μ_0, such that the tangent map induced from the inclusion i: $\mathsf{N} \to \mathsf{M}$ has the property that for each $\nu \in \mathsf{N}$, the tangent map $\mathscr{T}_\nu i$: $\mathscr{T}_\nu(\mathsf{N}) \to \mathscr{T}_\nu(\mathsf{M})$ is a topologically linear isomorphism of $\mathscr{T}_\nu(\mathsf{N})$ on $\mathscr{S}_\nu(\mathsf{N})$.

We state a version of Frobenius' local existence theorem which gives conditions on S guaranteeing its integrability.[35]

Theorem 2.1 (Frobenius): With M and S respectively a manifold and tangent subbundle as above, S is integrable iff for each point $\mu \in \mathsf{M}$ and all vector fields X and Y at μ which lie in S, the bracket $[X, Y]$ also lies in S. {It is to be understood here that X and Y are defined *on an open neighborhood of* μ. Also, in saying that X, for example, *lies in* S we mean that the image of each point μ of M under X lies in $\mathscr{S}_\mu(\mathsf{M})$. The bracket $[X, Y]$ is defined by $[X, Y](\nu) = X(Y(\nu)) - Y(X(\nu))$, where ν is any point in an open neighborhood of μ.} In other words, a necessary and sufficient condition for integrability of S is that its vector fields form a Lie algebra.

Definition[34]: The tangent subbundle S gives rise to a *regular foliation* of M if for any $\mu_0 \in \mathsf{M}$ there is a submanifold N (called a *leaf* of the foliation corresponding to μ_0) whose tangent bundle coincides with S.

D. Flows; operations involving vector fields

We can formalize the idea of flow by direct extension of finite-dimensional geometry. Thus, we say that a vector field X has *flow* F_t if $dF_t(\mu)/dt = X(F_t(\mu))$, $\forall \mu \in \mathsf{M}$. If $F_t(\mu)$ is defined $\forall t \in \mathbb{R}$, we say X has a *complete* flow, and the vector field itself is termed complete. The local existence and uniqueness theorem for flows in the infinite-dimensional case of interest to us can be found in Ref. 37.

For the infinite-dimensional geometry one needs to define Lie derivative and Lie bracket without reference to local coordinates and their differentials. As in the finite-dimensional case, this may be done in terms of flows.[35,36] For example, the *Lie derivative* at time t of a function $f: \mathscr{E} \to \mathbb{R}^1$, with respect to the vector field X with flow F_s, is specified by

$$\pounds_X f = \lim_{s \to t} (s-t)^{-1} [f(F_s(\phi)) - f(F_t(\phi))] ,$$

where $\phi \in \mathscr{E}$. The Lie derivative $\pounds_X Y$ of a vector field Y with respect to X may be defined similarly.[35] With these definitions one can show[35] that if (as in Sec. IV) we work on an analytic domain,[32] the expressions $\pounds_X f = Xf$ and $\pounds_X Y = [X,Y]$, familiar from finite-dimensional theory, will apply. For nested commutators, it will be convenient to use the notation $\mathrm{ad}_X^j Y = [X, \mathrm{ad}_X^{j-1} Y]$, $j \geqslant 1$, with $\mathrm{ad}_X^0 Y = Y$.

E. Densely defined vector fields

To this point we have implicitly or explicitly assumed that various quantities such as vector fields, flows, curves, etc., are well-defined on some open subset of the Banach space. It is useful to consider extensions of these quantities which are "densely defined."[37]

Definition: A *manifold domain* $\mathsf{D} \subset \mathsf{M}$ is a dense subset D in a manifold M, such that (a) D is also a manifold and (b) the inclusion map i: $\mathsf{D} \to \mathsf{M}$ is smooth and $\mathsf{T}i$ has dense range.

Definition[37]: A *densely defined vector field* is a cross-section map X: $\mathsf{D} \to \mathsf{T}(\mathsf{M})$ such that $X(\rho) \in \mathscr{T}_\rho(\mathsf{M}) \forall \rho \in \mathsf{D}$. A *flow* (alternatively termed an integral curve) for X then consists of a collection of maps F_t: $\mathsf{D} \to \mathsf{D}$, $t \in \mathbb{R}$, with the properties (a) $F_{t+s}(\rho) = F_t \circ F_s(\rho)$ and $F_0(\rho) = \rho$, $\forall \rho \in \mathsf{D}$, and (b) $dF_t(\rho)/dt = X(F_t(\rho))$, $\forall \rho \in \mathsf{D}$, the derivative being evaluated considering $F_t(\rho)$ as a curve in M. If in the latter specification $t \in \mathbb{R}$ is replaced by $t \geqslant 0$, we speak of a *semiflow* (or a semiintegral curve).

It is easily seen that all the definitions, properties, and theorems quoted in this section, although designed for an infinite-dimensional state space, are also applicable if the dimensionality is finite.

III. CONTROLLABILITY IN FINITE-DIMENSIONAL SPACES

The purpose of this section is to present the relevant existing results on finite-dimensional control systems, in a form which allows their ready extension to the quantum control problem on an analytic domain.

A. Problem formulation and basic definitions

Consider a control system whose state vector m evolves on a real analytic manifold M according to the dynamical law

$$\frac{d}{dt} m(t) = X_0(m(t)) + \sum_{l=1}^{r} u_l(t) X_l(m(t)) . \tag{3}$$

Here $X_0, X_1, \ldots, X_r$ are (possibly nonlinear!) vector fields on M, which resides in a *finite*-dimensional space. The admissible class of control functions $u_l(t)$ (the set $\{u_1(t), \ldots, u_r(t)\}$ being abbreviated as u) is again chosen to be the class of piecewise-constant functions from $[0,\infty)$ into $\mathbb{R}$. For emphasis we have changed notation relative to formulation (1), which refers to the more general situation where the state space may be infinite-dimensional.

Let $\mathscr{V}(\mathsf{M})$ be the set of all real, analytic vector fields on M. By the Frobenius theorem of Sec. IIC, $\mathscr{V}(\mathsf{M})$ in fact constitutes a Lie algebra over the reals. Supposing $\mathfrak{S}$ is a subset of $\mathscr{V}(\mathsf{M})$ and $\mathscr{L}_1$ and $\mathscr{L}_2$ are Lie subalgebras of $\mathscr{V}(\mathsf{M})$, it will be useful to introduce the following sets:

$$\mathfrak{S}(m) \equiv \{ Y(m) | Y \in \mathfrak{S} \} ,$$

$$\{\mathfrak{S}\}_{\mathrm{LA}} \equiv \mathscr{L}(\mathfrak{S}) \equiv \text{Lie algebra generated by } \mathfrak{S}$$

$$\text{(smallest Lie subalgebra of } \mathscr{V}(\mathsf{M}) \text{ containing } \mathfrak{S}),$$

$$[\mathscr{L}_1, \mathscr{L}_2] \equiv \{ [X,Y] | X \in \mathscr{L}_1, \quad Y \in \mathscr{L}_2 \} .$$

Assume that the solutions of the differential equation (3) are defined for all $t \geqslant 0$, and denote an individual solution by $m(m_o, u, t)$, where m_o is the initial state vector and $u = \{u_l\}$. An important definition follows.

Definition: Given $m_o, m_f \in \mathsf{M}$, we say that m_f is *reachable* from m_o at time t if there exists an admissible control u such that $m_f = m(m_o, u, t)$. The *reachable set* from n at time t, i.e., the set of points in M reachable at t, is symbolized by $\mathsf{R}_t(n)$. In addition, we introduce the reachable set from n in positive time: $\mathsf{R}(n) \equiv \cup_{t>0} \mathsf{R}_t(n)$.

The task at hand is to characterize these reachable sets, which, of course, determine the extent to which the system is controllable. It is by now well known[10,11,16–19] that the structures of $\mathsf{R}_t(n)$ and $\mathsf{R}(n)$ are intimately related to the Lie algebras

$$\mathscr{A} \equiv \{ X_0, X_1, \ldots, X_r \}_{\mathrm{LA}} ,$$

$$\mathscr{B} \equiv \{ X_1, X_2, \ldots, X_r \}_{\mathrm{LA}} ,$$

$$\mathscr{C} \equiv \{ \mathrm{ad}_{X_0}^j X_l | l = 1, \ldots, r; j = 0, 1, \ldots \}_{\mathrm{LA}} .$$

The essential relations will be traced in the next subsection. We note that $\mathscr{A}$, $\mathscr{B}$, and $\mathscr{C}$ are not necessarily finite-dimensional.

It is appropriate at this juncture to identify the primary sources of the essential ideas and results of geometric control theory in the finite-dimensional case. The work of Chow[3] stands as an obvious pinnacle of the field. In the pre-Chow era, we may point to studies of Caratheodory[39,40] and Radon.[41] (References 40 and 41 contain material on the calculus of variations which bears implicitly on controllability.) Subsequent to Chow, the primary literature includes the work of Hermann,[4,42] Sussmann and Jurdjevic,[10,11] Krener,[14] and Stefan.[24] Among the other articles on finite-dimensional geometric control theory cited above, we have found Refs. 16 and 19 particularly useful in formulating our outline of the subject, which follows.

B. Basic results on controllability (finite-dimensional state space)

The analysis of control system (3) rests on four fundamental theorems: the theorem of Frobenius (cf. Sec. IIC), Chow's theorem,[3] and two theorems due to Sussmann and Jurdjevic.[10,11]

1. Frobenius' theorem is, of course, fundamental to the geometric analysis of the control system (3), as already indicated above. To be given the control system normally means to be given the X_k, $k = 0,1,...,r$, and the $u_l(t)$, $l = 1,...,r$. Hence the Lie algebra constructed from the X_k and their repeated commutators is available, and one can use the theorem to circumscribe the analytic manifold on which the system is destined to evolve—presuming such a manifold exists. If the vector fields of $\mathscr{A} = \{X_0, X_1,...X_r\}_{\mathrm{LA}}$ are complete, then the local existence property guaranteed by the theorem as stated in Sec. IIC can be given a global extension in the following sense[16]: There will exist a maximal submanifold N of M containing the arbitrarily specified point $m_o \in$M (or $\mu_o \in$M in the more general context of Sec. II), such that $\mathscr{A}(n)$ (respectively $\mathscr{A}(\nu)$) spans the tangent space of N at each point n (respectively ν) of N.

2. To show how Chow's theorem comes into the picture, we pursue a line of reasoning[16] which begins with the desire to quantify changes in the dynamics produced by changes of the control $u(t)$. How can we represent the actual effect of the control in terms of $X_0, X_1,..., X_r$ and $u(t)$? We can appeal to the Campbell–Baker–Hausdorff formula. Consider $X, Y \in \mathscr{V}$(M), and denote their flows by X_t, Y_t, respectively. Then

$$X_{t_1} \circ Y_{t_2}(m) = Z_t(m)|_{t=1}, \tag{4}$$

where

$$Z = t_1 X + t_2 Y + \tfrac{1}{2} t_1 t_2 [X, Y] + \cdots \tag{5}$$

is a formal series which converges for t_1 and t_2 both in some neighborhood of 0.

In terms of the Campbell–Baker–Hausdorff formula (4)–(5), we may readily appreciate the role played by the Lie algebra of $\{X_0, X_1,...,X_r\}$ in the controllability problem. Let us temporarily focus on the modified control system governed by the dynamical equation

$$\frac{d}{dt} m(t) = \sum_{k=0}^{r} u_k(t) X_k(m(t)), \tag{6}$$

where all the u_k are piecewise-constant real functions of time. [Note the presence of the extra control factor $u_0(t)$.] Again the Campbell–Baker–Hausdorff formula may be used to trace the dynamics, and we infer that if $X \in \{X_0, X_1,...,X_r\}_{\mathrm{LA}}$ then $X_t(m_o)$ (also denoted simply $X_t m_o$) belongs to the reachable set of the (modified) system.

On the other hand, we can enlist the following argument[16] to circumscribe the set of reachable points of system (6). Assume that the vector fields of $\mathscr{V}$(M) are complete, and consider an arbitrary member X of this set. Then, for each t a mapping X_t of M onto itself is provided by the flow on M corresponding to the differential equation $dm/dt = X(m)$. Consider the group diff(M) of diffeomorphisms of M, i.e., the set of all C^∞ one-to-one and onto mappings of this C^∞ manifold onto itself, such that the inverse mappings are likewise C^∞. Let the smallest subgroup of diff(M) which contains X_t for all X in $\{X_k | k = 0,1,...,r\}$ be symbolized by $\{\{X_k\}_t\}_{\mathrm{G}}$. Now, we can easily see that any point in M expressible as $W m_o$, where $W \in \{\{X_k\}_t\}_{\mathrm{G}}$, can be reached from m_o along solution curves of (6). The indicated points are all like

$$(X_{\kappa_0})_{t_0} (X_{\kappa_1})_{t_1} \cdots (X_{\kappa_r})_{t_r} m_o ,$$

where $\{\kappa_0, \kappa_1,..., \kappa_r\} = \{0,1,...,r\}$; such points can certainly be attained by suitable switchings of the controls. One just sets $u_{\kappa_r} \equiv 1$ and the $u_{k \neq \kappa_r} \equiv 0$ for a time interval t_r, etc., finally setting $u_{\kappa_0} \equiv 1$ and the $u_{k \neq \kappa_0} \equiv 0$ for period t_0.

The obvious question is: How is the set of points $\mathrm{M}_1 \equiv \{ W m_o | W \in \{\{X_k\}_t\}_{\mathrm{G}}\}$ related to the set $\mathrm{M}_2 \equiv \{L m_o | L \in \{\{L_i\}_t\}_{\mathrm{G}}\}$, where $\{L_i\} = \{X_k\}_{\mathrm{LA}} = \mathscr{A}$. We know that M_1 is reachable, while M_2 promises to be a larger set. It is here that Chow's theorem may be brought to bear; in effect, it says that the sets M_1 and M_2 are *identical* (under some modest conditions). We state the theorem in the version given by Brockett.[16]

Theorem 3.1 (Chow): Suppose that $\{X_0(m), X_1(m),..., X_r(m)\}$ is an assembly of vector fields such that the elements of the Lie algebra $\mathscr{A}(m) = \{X_0(m), X_1(m),..., X_r(m)\}_{\mathrm{LA}}$ are (a) C^∞ on a C^∞ manifold M with dim $\mathscr{A}(m)$ constant on M or (b) analytic on an analytic manifold M. Then, in either case, given any point $m_o \in$M, there exists a maximal submanifold $\mathrm{M}' \subset \mathrm{M}$ containing m_o such that $\mathrm{M}_1 = \mathrm{M}_2 = \mathrm{M}'$. (*N.B.*: the arguments m are included in this statement to allow for the case that $X_0, X_1,..., X_r$ are nonlinear.)

We are thus able to draw some strong conclusions regarding the controllability of system (6) and the nature of its reachable set. But what about the system of immediate concern to us, namely (3)? Chow's theorem is not so incisive for this problem because it treats positive and negative times on an equal basis. The maximal submanifold M′ may contain points which can only be reached by moving *backwards* along the vector field $X_0(t)$. But in (3) there is no control factor $u_0(t)$ that we can set equal to -1, and such points are not actually reachable. Thus, in general, the reachable set $\mathrm{R}(m_o)$ for system (3) will be only a *proper subset* of the manifold $\mathrm{M}' = \mathrm{M}_2$ characterized by the Lie algebra $\mathscr{A} = \{X_0, X_1,..., X_r\}_{\mathrm{LA}}$.

3. Against the background of Chow's theorem, some limited progress toward the characterization of the reachable set $\mathrm{R}_t(m_o)$ for system (3) has been made by Sussmann and Jurdjevic.[10,11] To present their results, we formally introduce the *maximal integral manifold* $\mathrm{I}(\mathscr{W}, m)$ of $\mathscr{W}$ passing through $m \in$M, where $\mathscr{W}$ is an arbitrary subalgebra of $\mathscr{V}$(M). Explicitly, we mean by this that $\mathrm{I}(\mathscr{W}, m)$ is the largest connected submanifold N of M which contains m and has the property that for all $n \in$N, the tangent space to N at n is $\mathscr{W}(n)$. The existence of $\mathrm{I}(\mathscr{W}, m)$ follows from the global version of Frobenius' theorem. We also introduce, for $t > 0$, $\mathrm{I}_t(\mathscr{W}, m) \equiv \mathrm{I}(\mathscr{W}, X_{0t}(m))$. The relevant theorems are then:

Theorem 3.2 (Sussmann and Jurdjevic[10]): Let X_t and Y_t denote, respectively, the one-parameter flows of the vector fields $X, Y \in \mathscr{A}$. Then for all $m \in$M and $t \in \mathbb{R}$, $X_t(\mathrm{I}(\mathscr{C}, m)) = Y_t(\mathrm{I}(\mathscr{C}, m))$. In particular, $X_{0t}(\mathrm{I}(\mathscr{C}, m))$ is the unique maximal integral manifold of $\mathscr{C}$ through $X_{0t}(m)$. (*N.B.*: the definitions of Lie algebras $\mathscr{A}$, $\mathscr{B}$, $\mathscr{C}$ given in Sec. IIIA.)

Theorem 3.3 (Sussmann and Jurdjevic[10,17]): For all $m \in \mathsf{M}$ and $t > 0$, the reachable set $\mathsf{R}_t(m)$ of system (3) is a subset of $\mathsf{I}_t(\mathscr{C}, m)$; moreover, with respect to the topology of $\mathsf{I}_t(\mathscr{C}, m)$, the set $\mathsf{R}_t(m)$ is contained in the closure of its own interior.

The latter theorem tells us that $\mathsf{R}_t(m)$ has a nonempty interior in $\mathsf{I}_t(\mathscr{C}, m)$. This result ensues from the decomposition $\mathscr{A} \supset \mathscr{C} \supset \mathscr{B}$ of $\mathscr{A}$.

4. We are now equipped with the basic tools needed to pursue the controllability problem for system (3).

Definition: System (3) is said to be *strongly completely controllable* if $\mathsf{R}_t(m) = \mathsf{M}$ holds for all $t > 0$ and all $m \in \mathsf{M}$. If $\mathsf{R}(m) = \mathsf{M}$ holds for all m, the system is called *completely controllable*.

Following Kunita,[19] the key controllability results for our system will be framed in terms of families of vector fields drawn from $\mathscr{V}(\mathsf{M})$. In so doing, we make use of the following classification of vector fields, or more directly their associated integral curves.

Definition: With $m \in \mathsf{M}$, the integral curve $\{X_s(m), s \in \mathbb{R}\}$ is *attainable* [by system (3)] if both $X_t(m)$ and $X_{-t}(m)$ belong to $c\ell \mathsf{R}_t(m)$ for any $t > 0$ up to the closure time. If $X_t(m)$, but not necessarily $X_{-t}(m)$, belongs to $c\ell \mathsf{R}_t(m)$, we speak of *semiattainability*. On the other hand, if the more stringent condition is met that the full curve $\{X_s(m), s \in \mathbb{R}\}$ belongs to $c\ell \mathsf{R}_t(m)$, again for any $t > 0$, we say that $\{X_s(m), s \in \mathbb{R}\}$ is *strongly attainable*. *Strong semiattainability* of $\{X_s(m), s \in \mathbb{R}\}$ applies when the half curve $\{X_s(m), s \in \mathbb{R}^+\}$ belongs to $c\ell \mathsf{R}_t(m)$, $\forall t > 0$. The set of all vector fields on M whose integral curves are attainable (respectively, strongly attainable) is denoted by $\mathfrak{A}$ (respectively, $\mathfrak{A}_S$). The notation $\mathfrak{A}^+$ (respectively, $\mathfrak{A}_S^+$) is used for the corresponding semiattainable (respectively, strong semiattainable) case.

The above nomenclature is rooted in the nature of control systems, being manifestly predicated on the structure of the state-evolution equation, and in particular on what constraints are imposed on the control factors attached to $X_0, X_1, \ldots, X_r$. For example, set the u_l, $l = 1, \ldots, r$, identically zero and consider the autonomous system $dX_t/dt = X_0(X_t)$. It is seen that X_0 belongs to $\mathfrak{A}^+$ but not to $\mathfrak{A}$, since only one direction, and no control of amplitude, is associated with this vector field (i.e., $u_0 \equiv 1$). Now consider instead the system (3) with $X_0 \equiv 0$, thus the evolution equation $dm(t)/dt = \Sigma_{l=1}^r u_l X_l(m(t))$, and suppose the controls are restricted by $|u_l| = 1$ or 0. In this case we see that the vector fields $X_1, \ldots, X_r$ belong to $\mathfrak{A}$ because their effect on the dynamical state can be directed by $u_1, \ldots, u_r$; however, $X_1, \ldots, X_r \notin \mathfrak{A}_S$ because the amplitudes with which these vector fields enter the dynamical law cannot be manipulated with sufficient flexibility. On the other hand, when *no* constraints are imposed on the u_l, $l = 1, \ldots, r$ (apart from piecewise constancy), it is clear that $\mathscr{B} = \mathscr{L}(X_1, \ldots, X_r) \subset \mathfrak{A}_S$. For then $X_1, \ldots, X_r$ can always be "scaled" by appropriate controls $u_1(t), \ldots, u_r(t)$ in such a way that $m(t)$ reaches, at any chosen time t_f, any selected point on the manifold characterized, through the global version of Frobenius' theorem, by $\mathscr{B}$.

Besides the concept of attainable, semi-attainable, etc. sets, it is convenient to introduce the following notation. Let $\mathfrak{B}$ be a subset of $\mathscr{V}(\mathsf{M})$ and X an element of $\mathscr{V}(\mathsf{M})$. For a given positive integer q, consider the set of vector fields $\mathrm{ad}_{X^{(1)}}^{i_1} \cdots \mathrm{ad}_{X^{(p)}}^{i_p} X$ such that $i_1 + \cdots + i_p = q$, where $X^{(1)}, \ldots, X^{(p)}$ are mutually commuting, complete vector fields belonging to $\mathfrak{B}$. Denote the collection of *all* vector fields constructed in this manner, allowing for all qualifying choices of $\{X^{(1)}, \ldots, X^{(p)}\}$ in $\mathfrak{B}$, where p is to be varied also, by $\mathrm{ad}_{\mathfrak{B}}^{(q)} X$. The subset of $\mathrm{ad}_{\mathfrak{B}}^{(q)} X$ such that at least one of the indices $i_1, \ldots, i_p$ is odd, will be designated odd $\mathrm{ad}_{\mathfrak{B}}^{(q)} X$. [The basic reason we are interested in odd $\mathrm{ad}_{\mathfrak{B}}^{(q)} X$ is that it belongs to $\mathfrak{A}_S$, provided $X \in \mathfrak{A}^+$ and $X^{(1)}, \ldots, X^{(p)} \in \mathfrak{A}_S$ (Ref. 19).]

Two important theorems on the controllability of system (3) may now be established. Proofs are given in Refs. 19 and 43. It is assumed that $\dim \mathsf{M} = d < \infty$.

Theorem 3.4 (Kunita[19]): (i) If $\dim \mathfrak{A}_S(m) = d$ holds for all $m \in \mathsf{M}$, then system (3) is strongly completely controllable. (*N.B.*: $\mathfrak{A}_S$ is a Lie algebra.)

(ii) If $\dim \mathscr{L}(\mathfrak{A})(m) = d$ holds for all $m \in \mathsf{M}$, then system (3) is completely controllable.

Theorem 3.5 (Kunita[19]): Assume that for control system (3) one can find a sequence of sets $\mathfrak{B}_j$ of vector fields, $j = 0, 1, 2, \ldots$, with ordering $\mathfrak{B}_0 \subset \mathfrak{B}_1 \subset \mathfrak{B}_2 \subset \cdots$, which meet the following two criteria:

(i) $\mathfrak{B}_0 \subset \mathscr{B} = \mathscr{L}(X_1, \ldots, X_r)$;

(ii) for each value of the index j there exists a positive integer q_j such that $\mathrm{ad}_{\mathfrak{B}_j}^{(q_j+1)} X_0 \subset \mathscr{L}(\mathfrak{B}_j)$ and $\mathfrak{B}_{j+1} \subset \mathscr{L}(\mathfrak{B}_j$, odd $\mathrm{ad}_{\mathfrak{B}_j}^{(q_j)} X_0)$. It follows that $\mathscr{L}(\cup_{j=0}^{\infty} \mathfrak{B}_j) \subset \mathfrak{A}_S$. If in fact $\dim \mathscr{L}(\cup_{j=0}^{\infty} \mathfrak{B}_j)(m) = d$ holds for all $m \in \mathsf{M}$, system (3) is strongly completely controllable on M.

Corollary 3.5.1 (Kunita[19]): If $\dim \mathscr{C}(m) = d$ holds for all $m \in \mathsf{M}$ and $[\mathscr{C}, \mathscr{B}] \subset \mathscr{B}$, system (3) is strongly completely controllable.

These last two theorems summarize the main results from finite-dimensional control theory which we would like to extend to quantum dynamics. However, such extensions—to the extent that they are possible—necessitate careful attention to the domain problem arising from the infinite dimensionality of the quantum state space.

IV. CONTROLLABILITY OF QUANTUM-MECHANICAL SYSTEMS

Let us return now to the quantum-mechanical control problem formulated in Sec. I. Since in this case $H_0, H_1, \ldots, H_r$ of (1) must be linear, skew-Hermitian operators on a Hilbert space $\mathscr{H}$ and the $u_l(t)$ are piecewise-constant by assumption, there will be associated, with the quantum dynamics, a Lie group Γ whose elements may be represented by unitary operators on $\mathscr{H}$. The usual statistical interpretation of the state vector (wave function) $\psi(t)$ is reflected in its unitary evolution. The scalar product of vectors ϕ_1, ϕ_2 in the Hilbert space $\mathscr{H}$ is denoted $\langle \phi_1 | \phi_2 \rangle$. Imposing unit norm at the initial time $t = 0$, we have $\langle \psi(t) | \psi(t) \rangle = 1\ \forall t$; i.e., the dynamics unfold on the unit sphere of $\mathscr{H}$, denoted $\mathsf{S}_{\mathscr{H}}$.

A geometric description of quantum dynamics paralleling the description of Sec. III is facilitated by treating the state space $\mathscr{H}$ of the quantum system as a *real* Hilbert space. To this end, we may assert the formal decomposition

$\mathscr{H} = \mathscr{H}^R \times \mathscr{H}^I$, where $\mathscr{H}^R$ and $\mathscr{H}^I$ are real Hilbert spaces, isomorphic to one another. This decomposition is given meaning as follows. Consider an arbitrary state vector ϕ, interpreted to begin with as a vector in complex Hilbert space. We may choose some representation and identify real and imaginary parts, $\phi = \phi^R + i\phi^I$. Then ϕ^R is assigned to the space $\mathscr{H}^R$, i.e., $\phi^R \in \mathscr{H}^R$, while ϕ^I is assigned to $\mathscr{H}^I$. Thus ϕ is reinterpreted as a vector in a real Hilbert space constructed as the Cartesian product of $\mathscr{H}^R$ and $\mathscr{H}^I$. Correspondingly, we agree to compute the scalar product $\langle \phi_1 | \phi_2 \rangle$ as

$$\langle \phi_1 | \phi_2 \rangle = \langle \phi_1^R, \phi_2^R \rangle + \langle \phi_1^I, \phi_2^I \rangle ,$$

where $\langle \phi_1^R, \phi_2^R \rangle$ (respectively, $\langle \phi_1^I, \phi_2^I \rangle$) is the usual scalar product in the real Hilbert space $\mathscr{H}^R$ (respectively, $\mathscr{H}^I$). Since, in this work, we shall never have occasion to ascribe physical significance to the scalar product of two different vectors, these conventions will not bring us into conflict with those ordinarily adopted in quantum theory.[44] (For norms of state vectors, the two views obviously coincide.)

The above formal reinterpretation of $\mathscr{H}$, while entailing no loss of generality within the context of our aims, allows us to endow certain subsets of $\mathscr{H}$ with manifold structure. In particular, $S_{\mathscr{H}}$ is an infinite-dimensional submanifold of $\mathscr{H}$. For an explicit verification of the manifold character of $S_{\mathscr{H}}$, see Lang,[35] pp. 28–29. To see the geometric structure of $S_{\mathscr{H}}$, choose the local chart around $\chi_i \in S_{\mathscr{H}}$ as the projection of a neighborhood $U_i(\chi_i)$ to the space $\mathscr{H}_i \equiv \{ \eta | \langle \cdot \eta | \chi_i \rangle = 0, \eta \in \mathscr{H} \}$. The latter is manifestly a closed infinite-dimensional subspace of $\mathscr{H}$; moreover, $\mathscr{H}_i$ is isomorphic to $\mathscr{H}_j$ for all $\chi_i, \chi_j \in S_{\mathscr{H}}$.

A prominent feature of the quantum problem is that $H_0, H_1, \ldots, H_r$ are generally unbounded operators; it then becomes important to bring into play the notions of densely defined vector fields, and associated flows, curves, etc., introduced in Sec. II.

In this section, it is our primary task to show how results on controllability of finite-dimensional control systems, surveyed in Sec. III, can be generalized to infinite-dimensional, quantum-mechanical systems by exploitation of the properties of a certain type of manifold domain—an *analytic domain* $\mathscr{D}_\omega$. The existence of such a domain is assured by Nelson's theorem,[32] for a restricted but nontrivial class of skew-Hermitian operators $H_0, H_1, \ldots, H_r$. The conditions entering this theorem will appear rather restrictive, since they imply in particular that the Lie algebra $\mathscr{A} = \mathscr{L}(H_0, H_1, \ldots, H_r)$ associated with the quantum control system (1)–(2) is *contained* in the Lie algebra of operators on $\mathscr{H}$ obtained from the unitary representation of Γ. Still, the case of greatest relevance to engineering applications is included, namely, the harmonic oscillator with couplings to external classical fields. Moreover, an alternative formulation may be considered in which Nelson's theorem is not invoked: If one simply *assumes* the existence of an analytic domain $\mathscr{D}_\omega$, the extensions go through provided only that one imposes the additional assumption that the tangent space defined by $\mathscr{A}(\zeta)$ has constant finite dimension for all $\zeta \in S_{\mathscr{H}} \cap \mathscr{D}_\omega$. Within such a formulation the possibility remains open (at this point) that the Lie algebra $\mathscr{A}$ produced by $H_0, H_1, \ldots, H_r$ is *larger* than that derived from the group Γ, conceivably infinite-dimensional.

In either formulation, the problem of practical interest will of necessity be one of controllability on a *finite-dimensional* submanifold of the infinite-dimensional manifold $S_{\mathscr{H}}$ available to the normalized quantum state. This limitation of our treatment will be explained in Sec. IVC; in brief, controllability on $S_{\mathscr{H}}$ would entail infinite sequences of switchings of the $u_l(t)$.

A. Analytic vector and analytic domain

The reader should consult the original work of Nelson[32] for the underlying motivation and detailed development of the concepts of analytic vector and analytic domain (see also Ref. 33). In the interests of logical completeness, we should, nevertheless, recall the definition of analytic vector.

Definition: Let A be an operator in $\mathscr{H}$. An element ω of $\mathscr{H}$ is called an *analytic vector* for A if the series expansion of $(\exp sA)\omega$ has a positive radius of convergence, that is, if

$$\sum_{n=0}^{\infty} \frac{\|A^n \omega\|}{n!} s^n < \infty$$

for some real $s > 0$, where $\|A^n \omega\|$ is the Hilbert-space norm of $A^n \omega$.

Note that if A is bounded, all vectors of $\mathscr{H}$ are trivially analytic vectors for A; i.e., the concept of analytic vector becomes an incisive one only when dealing with unbounded operators—which, of course, are prevalent in quantum mechanics.

We should also state what it means to be an analytic vector for a Lie algebra.

Definition: A vector ω qualifies as an *analytic vector* for a Lie algebra $\mathscr{L}$ if for some $s > 0$ and some basis of the Lie algebra, say $\{H_{(1)}, \ldots, H_{(d)}\}$, the series

$$\sum_{n=0}^{\infty} \frac{1}{n!} \sum_{\substack{1 \leqslant i_1 < \cdots < i_d \leqslant d \\ n_1 + \cdots + n_d = n}} \|H_{(i_1)}^{n_1} \cdots H_{(i_d)}^{n_d} \omega\| s^n$$

converges.

The theorem of Nelson which is relevant to the present investigation is:

Theorem 4.1 (Nelson[32]): Let $\mathscr{L}$ be a Lie algebra of skew-Hermitian operators in a Hilbert space $\mathscr{H}$, the operator basis $\{H_{(1)}, \ldots, H_{(d)}\}$, $d < \infty$, of $\mathscr{L}$ having a common invariant dense domain. If the operator $T = H_{(1)}^2 + \cdots + H_{(d)}^2$ is essentially self-adjoint, then there exists a unitary group Γ on $\mathscr{H}$ with Lie algebra $\mathscr{L}$. Let $\overline{T}$ denote the unique self-adjoint extension of T. Then it furthermore follows that the analytic vectors of $\overline{T}$ (i) are analytic vectors for the whole Lie algebra $\mathscr{L}$ and (ii) form a set invariant under Γ and dense in $\mathscr{H}$.

The vital implication of this theorem for our work is that it establishes the existence, under definite conditions, of a dense domain $\mathscr{D}_\omega$ of analytic vectors which provides a foothold for the extension of the controllability results of Sec. III to the quantum problem (1)–(2). Indeed, the set of analytic vectors of $\overline{T}$ will constitute such a subspace $\mathscr{D}_\omega$ of $\mathscr{H}$. Making the obvious identification $\mathscr{L} = \mathscr{A}$, the elements of $\mathscr{A}$ are then seen to be densely defined vector fields on $\mathscr{D}_\omega \cap \mathsf{M}$, where M is a finite-dimensional manifold on which the system point evolves with time. (Such a manifold surely exists under the prevailing assumptions; we could, for example, choose it to be the manifold characterized by $\mathscr{A} = \{H_0, H_1, ..., H_r\}_{\rm LA}$ through Frobenius' theorem.) We also have the corresponding "densely defined" flows (cf. Sec. IIE).

The detailed reasoning runs as follows. Under the provisions of Nelson's theorem and by the nature of analytic vectors, we know that any element of the unitary group Γ associated with $\{H_0, H_1, ..., H_r\}$ can be represented locally in the exponential form $\exp Xt$, where X is some element of $\mathscr{A}$. Moreover, this exponential expression can be extended globally in t (see Refs. 32 and 33); in other words, if the elements of $\mathscr{A}$ are vector fields, they are in fact complete. That the elements of $\mathscr{A}$ do qualify as vector fields can be seen in terms of the definition given in Sec. IIB. First, $\gamma = (\exp Xt)\psi_o$ is a parametrized curve on manifold M with $\gamma(0) = \psi_o \in \mathsf{M}$. Hence $d(\varphi \circ \gamma)/dt\,|_{t=0}$ represents a tangent vector; choosing for φ the identity mapping, $X\psi_o$ represents a tangent vector at ψ_o on M. If, in particular, $\dim \mathscr{A}(\zeta) = \dim(\mathsf{M} \cap \mathscr{D}_\omega) = d < \infty$, $\forall \zeta \in \mathsf{M} \cap \mathscr{D}_\omega$, then it is sufficient to use $\mathscr{A}$ to characterize the tangent space $\mathscr{T}_\zeta(\mathsf{M})$ to M at ζ, and the tangent bundle $\mathsf{T}(\mathsf{M}) = \cup_{\zeta \in \mathsf{M} \cap \mathscr{D}_\omega} \mathscr{T}_\zeta(\mathsf{M})$. Referring now to the definition of vector field (and the definition of densely defined vector field, Sec. IIE), the elements X of $\mathscr{A}$ assuredly qualify as (densely defined) vector fields, since we may associate with each a mapping X: $\mathsf{M} \cap \mathscr{D}_\omega \rightarrow \mathsf{T}(\mathsf{M})$, with $X(\zeta) = (\zeta, X\zeta)$, $\zeta \in \mathsf{M} \cap \mathscr{D}_\omega$. In fact, each X is an *analytic vector* field on $\mathsf{M} \cap \mathscr{D}_\omega$ since φ is taken as the identity.

B. Analytic controllability

With an analytic domain at our disposal, it is advantageous to modify the notion of controllability, as follows.

Definition: Assuming that an analytic domain exists, system (1)–(2) is called *strongly analytically controllable* on $\mathsf{M} \subseteq \mathsf{S}_{\mathscr{H}}$ if $\mathsf{R}_t(\zeta) = \mathsf{M} \cap \mathscr{D}_\omega$ holds for all $t > 0$ and all $\zeta \in \mathsf{M} \cap \mathscr{D}_\omega$. If $\mathsf{R}(\zeta) = \mathsf{M} \cap \mathscr{D}_\omega$ holds for all $\zeta \in \mathsf{M} \cap \mathscr{D}_\omega$, the system is termed *analytically controllable on* M.

Within the formulation set up in Sec. IVA, in which we appeal to Nelson's theorem, we can choose M as the closure of the set $\{e^{s_0 H_0} e^{s_1 H_1} \cdots e^{s_r H_r} \psi_o,\ s_k \in \mathbb{R},\ k = 0,1,...,r\}$; this is certainly the maximal manifold on which the system will evolve from $\psi_o \in \mathsf{M} \cap \mathscr{D}_\omega$. From previous considerations we know that M is necessarily a finite-dimensional submanifold of $\mathsf{S}_{\mathscr{H}}$, that $H_0, H_1, ..., H_r$ are densely defined vector fields on $\mathsf{M} \cap \mathscr{D}_\omega$, which is, of course, dense in M, and that the tangent space of $\mathsf{M} \cap \mathscr{D}_\omega$ at ζ is characterized by $\mathscr{A}(\zeta)$, $\forall \zeta \in \mathsf{M} \cap \mathscr{D}_\omega$. If $\mathscr{A}(\chi)$ is of dimension d, for all $\chi \in \mathsf{S}_{\mathscr{H}} \cap \mathscr{D}_\omega$, we see that $\mathsf{S}_{\mathscr{H}}$ has been partitioned into a foliation with d-dimensional regular manifolds as leaves.

We are now ready to pursue the question of analytic controllability on M, in analogy with the treatment of Sec. III. On $\mathsf{M} \cap \mathscr{D}_\omega$, the flows of vector fields of $\mathscr{A}$ take exponential form, by virtue of the properties of an analytic domain. Hence a Taylor expansion is always well defined for any such flow. Consequently, the *Campbell–Baker–Hausdorff* formula applies, making available computational techniques which parallel those employed for the finite-dimensional state space. (The only distinction is that the norm is now calculated in Hilbert space.) At the same time, the *Frobenius theorem* stated in Sec. IIC is also valid with respect to $\mathscr{D}_\omega$, i.e., with M replaced by $\mathsf{M} \cap \mathscr{D}_\omega$. What about Chow's theorem? In the general infinite-dimensional case, the validity of this theorem is questionable. To see that it may be carried over to the present context, consider that the proof of the theorem (see, for example, Refs. 10 and 11) is based on (i) a paracompact topology for the manifold in question (here, $\mathsf{M} \cap \mathscr{D}_\omega$), (ii) finite dimensionality of the tangent space of that manifold, and (iii) the Campbell–Baker–Hausdorff formula. We have already seen that it is legitimate to invoke (iii), while it is well known that the submanifolds of a normed topological space (like $\mathscr{H}$) are always paracompact with respect to the relative topology. The crucial prerequisite is then (ii); but this property is intrinsic to our formulation based on Nelson's theorem. Thus, Chow's theorem does indeed hold within our restricted treatment of the quantum control problem. To be more specific, case (b) of the theorem as stated in Sec. IIIB applies, with $\mathsf{M} \cap \mathscr{D}_\omega$, $\{H_0, H_1, ..., H_r\}$, ψ, and ψ_o playing the roles of M, $\{X_0, X_1, ..., X_r\}$, m, and m_o, respectively.

Having these basic tools at our command it is routine to generalize the remaining results for the finite-dimensional control problem (3) to the quantum case, while exercising due care with regard to domains, norms, and limits. The details of this process, available in Ref. 43, are too lengthy to reproduce here. The upshot is that so far as Theorems 3.2 and 3.3 (Sussmann and Jurdjevic) are concerned, m goes over to ψ and M to $\mathsf{M} \cap \mathscr{D}_\omega$, and, of course, X_k is replaced by H_k, $k = 0,1,...,r$, in forming the Lie algebras $\mathscr{A}$ and $\mathscr{C}$. (*N.B.*: $\mathscr{V}(\mathsf{M})$ is reinterpreted as the set of all real, analytic vector fields on $\mathsf{M} \cap \mathscr{D}_\omega$.) The important results of Kunita are also readily adapted to the quantum problem, by making the same replacements. Because of its role in the examples to be presented in Sec. V, we recast Corollary 3.5.1 explicitly in these terms.

Corollary 3.5.1′: Let $\mathscr{C} = \{\mathrm{ad}^j_{H_0} H_l \,|\, l = 1,...,r;\ j = 0,1,\cdots\}_{\rm LA}$ be the ideal in $\mathscr{A} = \{H_0, H_1, ..., H_r\}_{\rm LA}$ generated by $H_1, ..., H_r$. Suppose that $\dim \mathscr{C}(\zeta) = d < \infty$, $\forall \zeta \in \mathsf{M} \cap \mathscr{D}_\omega$, and that $[\mathscr{C}, \mathscr{B}] \subset \mathscr{B}$. The quantum control system is then strongly analytically controllable on M.

The "practical" implication of this corollary is that (assuming the requisite conditions are met) we can always control the system so the state ψ, starting at any point $\psi_o \in \mathsf{M} \cap \mathscr{D}_\omega$, arrives arbitrarily close to any desired point in M after any chosen time interval t. Consequently, the expectation value of any observable quantity can be made to approach arbitrarily closely the expectation value of that quantity in any prescribed state vector in $\mathsf{M} \subset \mathscr{H}$, at any $t > 0$.

C. Controllability on $\mathsf{S}_{\mathscr{H}}$

Since Nelson's theorem requires that $\{H_0, H_1, ..., H_r\}$ gives rise to a finite-dimensional Lie algebra, it is apparently *not* possible to control the system on the unit sphere $\mathsf{S}_{\mathscr{H}}$ (i.e., with $\mathsf{M} = \mathsf{S}_{\mathscr{H}}$ in the definition of analytic controllability) if that theorem is in force. This is indeed the situation, the manifold M which enters the results of Sec. IVB being necessarily finite-dimensional. A more concise formal statement is given below.

Theorem 4.2: If $\{H_0,H_1,...,H_r\}$ generates a d-dimensional Lie algebra $\mathscr{A}$ which admits an analytic domain $\mathscr{D}_\omega$, the quantum system is not analytically controllable on $S_{\mathscr{H}}$ if d is finite.

Proof: By the properties of an analytic domain, there exists a connected, d-dimensional Lie group Γ with Lie algebra $\mathscr{A}$, the elements of Γ being constructed as $G = \exp X$ from members X of $\mathscr{A}$. Moreover, Γ can be chosen to act on $S_{\mathscr{H}} \cap \mathscr{D}_\omega$ according to $G(\xi) = (\exp X)\xi, \xi \in S_{\mathscr{H}} \cap \mathscr{D}_\omega$. Let $\mathscr{T}$ be an e-dimensional tangent subspace of $S_{\mathscr{H}}$ at ξ, and let P: $\mathscr{H} \to \mathscr{T}$ be the corresponding orthogonal projection from $\mathscr{H}$. Then $P(G\xi)$ defines a map from the d-dimensional Lie group Γ into the e-dimensional tangent subspace $\mathscr{T}$. This map cannot be onto if $e > d$. Further, since H_0 does not enter with an adjustable control factor $u_0(t)$, the dynamical semigroup Γ_s of the quantum system (1)–(2) is contained in the group Γ. Accordingly, if (as has been shown) Γ is not sufficiently rich to steer the state trajectory into all directions of $\mathscr{T}$, neither is Γ_s, and we conclude that the system is not analytically controllable on $S_{\mathscr{H}}$.

Corollary 4.2.1: If the quantum system is analytically controllable on $S_{\mathscr{H}}$, then $\mathscr{A}$ must be infinite-dimensional.

Proof: Direct observation.

Remark: In the case that $\mathscr{A}(\xi)$ is infinite-dimensional for all $\xi \in S_{\mathscr{H}} \cap \mathscr{D}_\omega$, an *arbitrary* flow of Γ would have the form $G(\xi) = [\Pi_j \exp s_j X^{(j)}]\xi, X^{(j)} \in \mathscr{A}, s_j \in \mathbb{R}, \{j\}$ infinite. In other words, if $\mathscr{A}(\xi)$ is infinite-dimensional, an infinite sequence of switchings would, in general, be required to build an element of Γ_s. Thus, within the context of piecewise-constant controls, practical realization of complete control of the quantum system (in the sense of analytic or strong analytic controllability on $S_{\mathscr{H}}$) is out of the question. Accordingly, our efforts have focused on the issue of controllability on finite-dimensional submanifolds of $S_{\mathscr{H}}$.

V. EXAMPLES

Example 1: In the context of a position or x representation[44] for state vectors and operators of $\mathscr{H}$, $x \in \mathbb{R}^1$, define

$$K_\pm = \pm \frac{1}{\sqrt{2}}\left(\frac{d}{dx} \mp x\right), \quad K_3 = -\frac{1}{2}\frac{d^2}{dx^2} + \frac{x^2}{2}, \tag{7}$$

together with $E =$ identity operator. The operators $-iK_3$, $K_+ - K_-$, and $i(K_+ + K_-)$ are skew-Hermitian, and the Lie bracket among them is specified through[45]

$$[K_3, K_\pm] = \pm K_\pm, \quad [K_+, K_-] = -E. \tag{8}$$

Making the identifications $H_0 = -iK_3$, $H_1 = K_+ - K_-$, and $H_2 = i(K_+ + K_-)$, we consider the system

$$\frac{d}{dt}\psi(t) = \{-iK_3 + u_1(t)[K_+ - K_-] + u_2(t)[i(K_+ + K_-)]\}\psi(t), \quad \psi(0) = \psi_o. \tag{9}$$

[For notational convenience we suppress, in (9), the fact that $\psi(t) = \psi(x;t)$ depends on the variable x, and that the derivatives entering should actually be partial derivatives.] The Lie algebra $\mathscr{L}(-iK_3, K_+ - K_-, i(K_+ + K_-)) = \mathscr{A}$ has basis $-iK_3$, $K_+ - K_-$, $i(K_+ + K_-)$, iE over $\mathbb{R}^1$, and it is well known[33,45] that there is a common dense invariant domain—an analytic domain $\mathscr{D}_\omega$—for these operators, spanned by analytic functions $\phi_n(x)$. Explicitly,

$$\phi_n(x) = \pi^{-1/4}(n!)^{1/2}(-1)^n 2^{-n/2} \exp[-x^2/2] h_n(x), \quad n = 0,1,2,...,\infty, \tag{10}$$

where the $h_n(x)$ are Hermite polynomials. As basis of the Lie algebra $\mathscr{L}(K_+ - K_-, i(K_+ + K_-)) = \mathscr{B}$ one has simply $K_+ - K_-, i(K_+ + K_-), iE$. This basis is in fact shared by the ideal $\mathscr{C}$ in $\mathscr{A}$ generated by $H_1 = K_+ - K_-$ and $H_2 = i(K_+ + K_-)$. Thus the Lie algebras $\mathscr{B}$ and $\mathscr{C}$ coincide, and the property $X \in \mathscr{C}$, $Y \in \mathscr{C} \Rightarrow [X,Y] \in \mathscr{B}$ emerges trivially. Furthermore, we verify from (7) and (10) [or (8)] that $\dim \mathscr{A}(\omega) = \dim \mathscr{B}(\omega) = \dim \mathscr{C}(\omega) = d = 3$ for all $\omega \in \mathscr{D}_\omega$; moreover, $\dim \mathrm{I}(\mathscr{C}, \xi) = 3$ for all $\xi \in S_{\mathscr{H}} \cap \mathscr{D}_\omega$. The essential relations are

$$K_+\phi_n = (n+1)^{1/2}\phi_{n+1}, \quad K_-\phi_n = n^{1/2}\phi_{n-1},$$
$$K_3\phi_n = (n + \tfrac{1}{2})\phi_n, \quad E\phi_n = \phi_n. \tag{11}$$

[For the special case $\omega = \phi_o$, we have $K_-\omega = 0$. However, even in that case we obtain in effect three linearly independent vectors upon application of the basis operators $-iK_3$, $K_+ - K_-$, $i(K_+ + K_-)$, iE, since our Lie algebras are defined over the reals.]

By virtue of the properties just displayed, Corollary 3.5.1′ (stated in Sec. IVB) comes into play, and we may conclude that (i) the reachable set of ψ_o in $S_{\mathscr{H}} \cap \mathscr{D}_\omega$ is given by $\mathrm{I}(\mathscr{C}, \psi_o) = \mathrm{I}(\mathscr{B}, \psi_o)$ for $\psi_o \equiv \psi(0) \in \mathrm{span}\{\phi_n(x), n = 0,1,2,...,\infty\}$ and (ii) putting $\mathsf{M} = c\ell\,\mathrm{I}(\mathscr{B}, \psi_o)$, the system is strongly analytically controllable on M.

At a more intuitive level, one can argue from (11) that the dynamical effect of $H_0 = K_3$ can be cancelled by that of some input which dominates $\mathscr{B}$; this implies strong analytic controllability, checking the implication of Corollary 3.5.1′.

Physically, the state-evolution equation of (9), multiplied by i, may be interpreted as the Schrödinger equation governing the dynamics of a one-dimensional quantum oscillator coupled independently via its momentum and position operators to external controls (fields) $u_1(t)$ and $u_2(t)$, respectively. The operator K_3 represents the energy of the uncoupled oscillator, while K_+ and K_- serve, respectively, as creation and destruction operators for harmonic excitations.

Example 2: The commutation relations (8) bring to mind the commutation relations for the spherical components of the angular momentum operator **J**. Given the Cartesian components J_x, J_y, J_z of **J**, we form the spherical components $J_\pm = J_x \pm iJ_y$, $J_3 = J_z$ and obtain[45]

$$[J_3, J_\pm] = \pm J_\pm, \quad [J_+, J_-] = 2E. \tag{12}$$

We note that (12) coincides with (8) *except* for the presence of a factor 2 on the right-hand side of the last relation, instead of a factor -1. It is evident that one can go on to formulate simple examples of the quantum controllability problem based on the Lie algebra $\mathscr{L}(-iJ_x, -iJ_y, -iJ_z)$ of the angular momentum operators.

In particular, one might set $H_0 = -iJ_z$, $H_1 = -iJ_x$, and $H_2 = -iJ_y$, and consider the system equation

$$\frac{d}{dt}\psi(t) = \{-iJ_3 + u_1(t)[J_+ - J_-] + u_2(t)[i(J_+ + J_-)]\}\psi(t),$$
$$\psi(0) = \psi_o, \tag{13}$$

wherein we revert to our earlier interpretation of $\psi(t)$ as an element of the abstract state space. The resemblance between problems (13) and (9) is strong; for instance, we find the corresponding properties that $\mathscr{A}$ has basis $-iJ_z$, $-iJ_x$, $-iJ_y$, $-iE$, and that $\mathscr{B}$ and $\mathscr{C}$ share the basis $-iJ_x$, $-iJ_y$, $-iE$. On the other hand, an important distinction must be recognized. In the present case there exists a Casimir operator, i.e., a (non-trivial) function of base elements of the Lie algebra $\mathscr{A}$ which commutes with all base elements, whereas in Example 1 there is no such (nontrivial) operator. Here the Casimir operator is, of course, the square of the angular momentum, $\mathbf{J}^2 = J_x^2 + J_y^2 + J_z^2$. Thus, if we suppose that the state of the quantum system is initially in a subspace of eigenvalue $j(j+1)$ of $\mathbf{J}^2$, where $j \geqslant 0$ is integral or half-odd integral, it will always remain in that subspace. Having chosen a definite value of j, and having agreed that J_x, J_y, J_z and functions of them are the *only* relevant observables [as is the case for the particular system (13) and notably for situations in which only spin degrees of freedom are manifest], we have a problem involving a *finite-dimensional* state space χ_j, of dimension $2j+1$. Accordingly, the results of Sec. IIIB 3–4 are directly applicable, and, taking account of the skew-Hermitian nature of H_0 and the H_l, it follows that strong complete controllability prevails on the unit sphere in χ_j. Numerous explicit physical examples of this sort are encountered in the fields of atomic- and molecular-beam experiments and magnetic resonance; for archetypal cases, see Ref. 46.

Example 3: Consider the system

$$i\frac{d}{dt}\psi(t) = [P_1^2 + P_2^2 + u_1(t)P_1 + u_2(t)P_2]\psi(t),$$
$$\psi(0) = \psi_o, \tag{14}$$

where P_1 and P_2, in the x_1x_2 representation, $x_1x_2 \in \mathbb{R}^2$, have the modes of action $-i\partial/\partial x_1$ and $-i\partial/\partial x_2$, respectively. The common eigenfunctions of the commuting operators P_1, P_2 do not lie in $L^2(\mathbb{R}^2)$ and so do not qualify as representatives of Hilbert-space state vectors; however, we know from the theory of Fourier transforms that these common eigenfunctions span $L^2(\mathbb{R}^2)$ in the sense of integral superpositions. In terms of such Fourier-integral superpositions, one may in fact define a common, dense, invariant domain of $L^2(\mathbb{R}^2)$ for the unbounded operators $H_0 = -i(P_1^2 + P_2^2)$, $H_1 = -iP_1$, and $H_2 = -iP_2$. Moreover, the solution of the Schrödinger dynamical problem (14), with initial value ψ_o in the latter domain, can be expressed in exponential form. The foregoing heuristic sketch indicates that it is possible to construct a suitable analytic domain $\mathscr{D}_\omega$ for the control problem specified by (14). A rigorous construction can be formulated in terms of Nelson's theorem as stated in Sec. IV, with $T = (P_1^2 + P_2^2)^2 + P_1^2 + P_2^2$.

Now let $\psi_{k_1k_2}$ be a common eigenvector of P_1 and P_2 with respective eigenvalues k_1 and k_2, or, more properly, a wave packet or eigendifferential[44] constructed as an integral superposition of eigenvectors of these operators with respective eigenvalues lying in arbitrarily narrow intervals centered on k_1, k_2. We are faced in this example with a degenerate situation in which H_0, H_1, and H_2 all commute with one another. Thus, $[\mathscr{B}, \mathscr{C}]$ collapses to the null set. Consequently, the chosen state $\psi_{k_1k_2}$ belongs to the reachable set $\mathsf{R}(\psi_o)$ only if $\psi_o = c(0)\psi_{k_1k_2}$, $|c(0)|^2 = 1$; under this condition the system always stays on the one-dimensional manifold defined by $c(t)\psi_o$, with $|c(t)|^2 = 1$. The controls $u_1(t)$ and $u_2(t)$ can at most change the phase of the state and hence are ineffectual, since all physical predictions are independent of this phase.

One may of course interpret the Schrödinger equation of (14) as that for two equal-mass particles moving in one dimension. The particles do not interact with one another, but are coupled independently via their respective momenta to controls (fields) $u_1(t)$ and $u_2(t)$.

VI. SUMMARY AND OUTLOOK

It has been our aim to lay a foundation for the concept of controllability of quantum-mechanical systems. Referring to expressions (1) and (2), a quantum control system is characterized by its internal Hamiltonian $H_0' = i\hbar H_0$, which is the infinitesimal generator of the free evolution of the quantum object, together with the operators $H_1' = i\hbar H_1, \ldots, H_r' = i\hbar H_r$, which couple that object to external controls of respective amplitudes $u_1(t), \ldots, u_r(t)$. Working within traditional quantum theory, where the H_k $(k = 0,1,\ldots,r)$ are linear, skew-Hermitian operators, we have succeeded in deriving conditions for global controllability on a certain finite-dimensional submanifold of the physical Hilbert space $\mathscr{H}$. The cornerstone of the associated analysis is an analytic domain $\mathscr{D}_\omega$, which we presume to exist for the given operators. The results we have obtained are natural extensions of well-known systems-theoretic results in finite-dimensional state space (drawn especially from Refs. 10, 11, 14, 16, 17, and 19). Generalizations to nonlinear versions of the quantum control problem (corresponding to nonlinear extensions of quantum theory) have not been considered here, but some results on local controllability in the context of nonlinear operators H_k have been derived in Ref. 43. The present work on the quantum controllability problem has provided a background for investigation of the invertibility of quantum-mechanical systems[47] and the formulation of a quantum nondemolition filter.[48,49]

Still, only a modest beginning has been made toward achieving the larger goal of a comprehensive theory of quantum control and filtering. The following problems, among others, await concerted effort:

(i) Generalization of the present treatment of quantum controllability to a less restrictive scene of action than a domain of analytic vectors—for example, a domain composed of vectors of $\mathscr{H}$ for which the orbits are infinitely differentiable functions of the group parameters.

(ii) Investigation of controllability for the case of control functions $u_l(t)$ belonging to $L^2(\mathbb{R})$.

(iii) Study of a controlled version of the Schrödinger equation for the time evolution of the density operator,[44] so as to extend control theory to the realm of quantum statistical mechanics.

(iv) Adaptation of the notions of observability, identification, realization, and feedback to the quantum setting.

It is evident that powerful mathematical techniques must be invoked to carry through this program; moreover, one must confront the profound conceptual obstacles intrinsic to the quantum measurement process.[50–52]

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