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Control of Quantum Systems

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Abstract

A quantum system subject to external fields is said to be controllable if these fields can be adjusted to guide the state vector to a desired destination in the state space of the system. Fundamental results on controllability are reviewed against the background of recent ideas and advances in two seemingly disparate endeavors: (i) laser control of chemical reactions and (ii) quantum computation. Using Lie-algebraic methods, sufficient conditions have been derived for global controllability on a finite-dimensional manifold of an infinite-dimensional Hilbert space, in the case that the Hamiltonian and control operators, possibly unbounded, possess a common dense domain of analytic vectors. Some simple examples are presented. A synergism between quantum control and quantum computation is creating a host of exciting new opportunities for both activities. The impact of these developments on computational many-body theory could be profound.

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I. INTRODUCTION

Since the birth of quantum theory, scientists have engaged in an abundance of experimental efforts to control quantum systems, with prominent successes in particle acceleration and detection, magnetic resonance, electron microscopy, solid-state electronics, and laser trapping. However, the need for a comprehensive theory of quantum control was not recognized until the beginning of the 1980's, when powerful concepts and methods from systems engineering were first integrated into the quantum framework [1–6]. The subject soon received a strong impetus from the prospects for optical control of chemical reactions opened by tremendous advances in laser technology. There followed a period of rapid development of techniques for practical control of molecular dynamics, including continuous-wave coherent control [7], dual-pulse control [8], optimal control [9,10], inverse control [11], and "closed-loop" learning control [12]. This work has already been the subject of several reviews [16,13–15,17].

Looking back to the origins of quantum control theory, it noteworthy that the seminal ideas of quantum information theory and quantum computation emerged during the same period [19–21]. The source of the vast potential of both quantum control and quantum computation stems from the superposition principle of quantum mechanics and in turn from the simple fact that "Hilbert space is a big place." The icon is the double-slit experiment, in which two quantum paths are generated and caused to produce a wave interference pattern. More specifically:

- In *quantum control* of molecular dynamics using lasers, one seeks to create two or more independent quantum pathways of the light-field–molecule system that interfere constructively or destructively so as to attain a specified target condition, e.g. a larger yield for one reaction product in preference to others. "Manipulation of the phases of molecular, atomic, and electronic systems, through the use of laser phase, provides a general paradigm for control of quantum dynamics." [22]

- Similarly, *quantum computation* exploits superposition to achieve massive parallelism and ideally an exponential speedup of processing. "A quantum computer obeys the laws of quantum mechanics, and its unique feature is that it can follow a superposition of [many!] computational paths simultaneously and yield a final state depending on the interference of these paths." [23].

Surprisingly, the intimate connection of these two developments has only recently been brought to the surface [15,25,24]. Nevertheless it is clear that quantum control, in the sense of implementing designated unitary transformations in the state space, is an essential ingredient of quantum computation; and on the other hand, quantum control theory will surely benefit from advances in quantum computing.

The mysteries and paradoxes of quantum mechanics, most especially those arising from superposition and entanglement (the double-slit experiment; Schrödinger's cat; the EPR paradox with its "spooky action at a distance") are being harnessed to create the advanced technologies of the future. We are reminded of science-fiction author Robert A. Heinlein's penetrating remark that "Any advanced technology is indistinguishable from magic."

II. CONTROLLABILITY 101

We begin our discussion of quantum dynamics and its control at a textbook level, then increase or decrease rigor as deemed convenient or appropriate. The solution of the time-dependent Schrödinger equation

$$i\hbar\dot{\psi}(t) = H\psi(t) \tag{1}$$

for the state vector $\psi(t)$ can be expressed in terms of a unitary transformation $\psi(t) = U\psi_0$ on the initial state $\psi(t=0) = \psi_0$. Importantly, for a Hamiltonian H that is not an explicit function of time, the unitary time-evolution operator U takes the exponential form

$$U(t,0) = \exp\left[-iHt/\hbar\right] . \tag{2}$$

Henceforth we take $\hbar = 1$.

To gain an intuitive grasp of the controllability problem, it is instructive to consider a Schrödinger equation of the type

$$i\dot{\psi}(t) = H\psi(t) = \sum_{i=1}^{r} u_i(t) H_i \psi(t)\,, \tag{3}$$

again with boundary condition $\psi(t=0) = \psi_0$, where the $u_i(t)$ are real control functions that can be turned on or off at will and the Hermitian control operators H_i are all time independent. Now let's go on a little trip, first here on Earth in a flat place like Holland and then in Hilbert space. Suppose in both cases there are only two controls, two possible "'directions" of motion (four when you count the possibilities of forward and backward motion). For the trip on Earth, go North for one hour, then West for one hour, then South for one hour, and finally East for one hour, maintaining a steady speed on each leg. You wind up where you started, so the succession of translations has not given anything new (this being no surprise, since translation is a commutative operation).

For the trip in Hilbert space, turn on H_2 for t units of time, then H_1 for t units, then $-H_2$ for t units, and finally $-H_1$ for t units (the minus signs come from the flexibility of the $u_i(t)$, which we take to be piecewise constant). In general, you do not wind up in the same place! The state vector will reach the point

$$\psi = \exp(iH_1 t)\exp(iH_2 t)\exp(-iH_1 t)\exp(-iH_2 t)\psi_0\,. \tag{4}$$

Expanding in the parameter t (which we may shrink toward zero), we have

$$\psi = \psi_0 + \frac{t^2}{2}[H_1, H_2]\psi_0 + O(t^3) = \exp\left([H_1, H_2]t^2/2\right)\psi_0 + O(t^3)\,. \tag{5}$$

If the commutator does not vanish, the alternating application of the two operators H_1 and H_2 at our disposal has given us a "new direction" in which we can move the solution – a new kind of rudder or oar for sailing the seas of Hilbert space.

Going to the case where the number r of controls i is arbitrary (but finite), it becomes apparent [26,27,24,29,28,25] that by selecting a sequence of unitary transformations each generated by a member of the given set $\{H_i, i = 1, \cdots, r\}$, one can achieve the effect of *any* Hamiltonian in the Lie algebra produced from the original set by an operation of repeated commutation. Denoting the skew-Hermitian counterpart $-iH_i$ of H_i by $\hat{H}_i$, this Lie algebra is the real linear vector space spanned by the operators $\hat{H}_i$ and their mutual commutators of all orders. We can clearly go anywhere in Hilbert space that can be reached through exponentiation of any member $\hat{L}_i$ of this Lie algebra:

$$\psi(t) = U(t,0)\psi_0 = e^{\hat{L}_i t}\psi_0 \,. \tag{6}$$

This result, rooted in the Baker-Campbell-Hausdorff formula [30] familiar to physicists, is well known in "classical" control theory [18] and provides the basis for geometric control. It is certainly at the heart of the original effort to extend classical controllability results to the quantum domain [3]. Moreover, it is the key ingredient of Lloyd's proof [27] that "almost all quantum logic gates are universal" (see also Deutsch and coworkers [21,31], Sleator and Weinfurter [32], and DiVicenzo [33]).

Let us take a moment to understand in broad terms what this last statement means. Consider a quantum computer that manipulates distinct quantum bits, or "qubits" (i.e., linear superpositions of definite "on" and "off" states, which might be represented by "up" and "down" states of a spin-half particle or the excited and ground states of an atom). Such a computer is said to be *universal* if, by implementing a finite sequence of *local operations*, it can perform an arbitrary unitary transformation over those variables with arbitrary precision. (This is equivalent to controllability in a finite-dimensional state space.) In particular, one can show that two-qubit CNOT gates, combined with single-qubit operations, can do the job. In this sense, the CNOT gate is itself said to be universal. A CNOT gate carries out the XOR operation: the XOR of two bits is the sum of their Boolean values, modulo 2. In a fascinating development, Gershenfeld and Chuang [34] have created a quantum CNOT gate in the laboratory by exploiting the interaction between the nuclear spins of the hydrogen and carbon atoms in chloroform molecules ($CHCl_3$) in a liquid sample subject to an external magnetic field. A sequence of two π-pulse radiofrequency signals flips the spin of the H nucleus (representing the target bit) *if and only if* the spin of the ^{13}C nucleus (the control bit) is parallel to the external field. This design provides the basis for a quantum computer controlled by nuclear magnetic resonance.

By a geometrical argument patterned after that sketched above, Lloyd [27] was able to show that "almost any quantum logic gate with two or more inputs is universal." If one can repeatedly apply a given control Hamiltonian to a system, which evolves autonomously between such applications, then provided that the Lie algebra generated by the control Hamiltonian and the unperturbed Hamiltonian H_0 closes on the full space of Hamiltonians for the system, one can build any desired unitary transformation on the system. "Essentially, any nontrivial interaction between quantum variables will do."

Against this background, we now resume the main line of development. For the control system based on (3), strong controllability results follow from classical control theory as developed by systems engineers and mathematicians [35,36,18]. Introduction of an additional term on the right-hand-side of Eq. (3) to describe autonomous motion driven by a "drift" Hamiltonian H_0 (which is *not* multiplied by a control function) complicates matters somewhat. However, this complication has been addressed explicitly by Lloyd [27] and Weaver [37] and less directly by Ramakrishna and coworkers [24,26].

The formulation of Ramakrishna and Rabitz [24] is conveniently succinct. They consider a system having an n-dimensional state space (where n is finite but otherwise arbitrary) and focus on the equation of motion of the time-development operator U that "evolves" the system state via $\psi(t) = U(t,0)\psi_0$:

$$\dot{U}(t,0) = \hat{H}_0 U(t,0) + \sum_{i=1}^{r} u_i(t) \hat{H}_i U(t,0)\,, \qquad U(0,0) = I\,. \tag{7}$$

Here U is a unitary $n \times n$ matrix (with I the $n \times n$ identity matrix), while $\hat{H}_0$ and the $\hat{H}_i$ are $n \times n$ skew-Hermitian matrices. The control functions $u_i(t)$ are assumed to be well enough behaved that the problem (7) always has a unique solution. The driftless case where $\hat{H}_0$ is absent, which corresponds to Eq. (3), is the one most commonly entertained in the theory of quantum computation. The system (7) is said to be *controllable* if the matrices $\hat{H}_0$, $\hat{H}_i$

and the control functions $u_i(t)$ allow every $n \times n$ matrix U to be reached in finite time.

Theorem [24]. A necessary and sufficient condition for the system (7) to be controllable is that the set comprised of $\hat{H}_0$ and the $\hat{H}_i$ $(i = 1, \ldots, r)$, together with all commutators and repeated commutators among these matrices (i.e., the Lie algebra generated by $\hat{H}_0$ and the $\{\hat{H}_i, , i = 1, \ldots, r\}$) equals *all* the $n \times n$ skew-Hermitian matrices. Additionally, when this condition is met, any unitary $n \times n$ matrix U can be constructed by choosing the control functions $u_i(t)$ to be piecewise-constant functions of the time.

Further definitive results for the finite-dimensional case have been derived [38].

The going gets tougher when the state-space becomes infinite-dimensional (a true Hilbert space) and especially when one must deal with unbounded operators and consider the control of dynamical states lying in the continuum. The next section deals with these cases, which, for brevity, we will refer to as continuous quantum systems, since they generally involve operators like x and p (position and momentum) with continuous spectra, as well as eigenstates that cannot be represented in Hilbert space. The existing results [3,28,42–45] are limited, but hardly trivial.

III. CONTROLLABILITY OF CONTINUOUS QUANTUM SYSTEMS

We consider a quantum system whose state $\psi(t)$ evolves from $\psi(t = 0) = \psi_0$ according to the Schrödinger equation

$$\dot{\psi}(t) = \left[\hat{H}_0 + \sum_{i=1}^{r} u_i(t)\hat{H}_i\right] \psi(t)\,, \tag{8}$$

which differs from Eq. (3) by the insertion of the usual term for autonomous evolution, or drift. The state space $\mathcal{H}$ can now be infinite-dimensional, and $\hat{H}_0$, $\hat{H}_1$, ..., $\hat{H}_r$ are linear, time-independent, skew-Hermitian operators in this space. Imposing $||\psi(t)|| = 1$, the system evolves on the unit sphere $S_{\mathcal{H}}$ in $\mathcal{H}$. As before, the u_i are real functions of t.

Eq. (8) provides the basis for a rather general control problem. In its purest form, the problem is to find a set $u(t)$ of controls $u_i(t)$ that steer the state of the system from ψ_0 at the initial time to a desired target state ψ_f at some later time t_f. One might alternatively seek controls that lead the state to a specified region of the state space, or one might prescribe a particular trajectory for $\psi(t)$ subsequent to $t = 0$. Thus the quantum control problem is intrinsically nonlinear in that the controls themselves, which multiply the state ψ in Eq. (8), may depend on the posed behavior of $\psi(t)$. However, systems engineers regard this a bilinear control problem: bilinear in ψ and the u_i.

Transference or extension of results on classical bilinear control systems and controllability (see, e.g., Chow [35], Sussmann and Jurdjevic [36], and Brockett [18]) is impeded not only by the infinite dimensionality of the state space $\mathcal{H}$ and the unit sphere $S_{\mathcal{H}}$, but also by the presence of unbounded operators such as x, $-i\partial_x$, and $-\partial_x^2$. These domain problems can be partially overcome if one assumes the existence of an *analytic domain* $\mathcal{D}_\omega$, a set of state vectors having three properties: (i) it is dense in the Hilbert space $\mathcal{H}$, (ii) it is invariant under the given operators $\hat{H}_i$ (with $i = 0, 1, \ldots, r$), and (iii) on it, the solution of the Schrödinger equation (8) can be expressed globally in exponential form. In simple terms, the availability of an analytic domain, in the context of piecewise-constant controls, allows one to write the evolution operator U corresponding to a Hamiltonian H in the familiar way, $U(t, 0) = e^{-iHt} = e^{\hat{H}t}$. (Strictly, it will also be necessary to invoke the Nuclear Spectral Theorem [39] and the construction of a rigged Hilbert space, to encompass states belonging to continuous spectra.)

Short of actually finding the controls producing a desired result, one can ask whether or not such controls exist at all. To address this existence issue systematically, we need to adopt precise definitions of *reachable sets* and *controllability*. The state $\psi(t) \in S_{\mathcal{H}}$ of the controlled system (8) evolves from ψ_o on a set M which forms a differentiable manifold, finite or infinite-dimensional [18]. (We note that $S_{\mathcal{H}}$ may itself be endowed with manifold structure.)

Def. Given ψ_o, $\psi_f \in$ M, we say that the state ψ_f is *reachable* from ψ_o at time $t_f > 0$ if there exists an admissible control $u(t)$ such that $\psi(t = t_f | u, \psi_o) = \psi_f$. The set of states reachable from ψ_o at time t_f is denoted $R_{t_f}(\psi_o)$. The set of states reachable from ψ_o at some positive time is $R(\psi_o) = \cup_{s>0} R_s(\psi_o)$.

Def. The control system is said to be *strongly completely controllable* if $R_t(\psi_o) = \mathrm{M}$ holds for all times $t > 0$ and all $\psi_o \in \mathrm{M}$. The system is *completely controllable* if $R(\psi_o) = \mathrm{M}$ holds for all $\psi_o \in \mathrm{M}$.

Accommodating the role to be played by the analytic domain, we introduce modified definitions of controllability:

Def. Let ψ_o be an *analytic vector* belonging to an *analytic domain* $\mathcal{D}_\omega$ that is dense in the state space. Then the control system (8) is *strongly analytically controllable* [respectively, *analytically controllable*] on $\mathrm{M} \subseteq S_{\mathcal{H}}$ if $R_t(\psi_o) = \mathrm{M} \cap \mathcal{D}_\omega$ holds for all $t > 0$ and all $\psi_o \in \mathrm{M} \cap \mathcal{D}_\omega$ [respectively, if $R(\psi_o) = \mathrm{M} \cap \mathcal{D}_\omega$ holds for all $\psi_o \in \mathrm{M} \cap \mathcal{D}_\omega$].

The existence of an analytic domain is guaranteed by *Nelson's Theorem* [39], if we choose to impose the associated conditions, which, as will now be revealed, are not especially restrictive from the physical standpoint.

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

With the identification $\mathcal{L} = \mathcal{A} \doteq \{\hat{H}_0, \hat{H}_1, ..., \hat{H}_r\}_{\mathrm{LA}}$, the elements of $\mathcal{A}$ become densely defined vector fields on $\mathcal{D}_\omega \cap \mathrm{M}$, where $\dim \mathrm{M} \cap \mathcal{D}_\omega = d < \infty$ and M is the finite-dimensional manifold on which the system point evolves with time [18]. The manifold M is given by the closure of the set $\{\mathrm{e}^{s_0 \hat{H}_{\alpha_0}} \mathrm{e}^{s_1 \hat{H}_{\alpha_1}} \cdots \mathrm{e}^{s_r \hat{H}_{\alpha_r}} \psi_o\}$, with $(\alpha_0, \alpha_1, \ldots, \alpha_r)$ any permutation of $(0, 1, \ldots, r)$ and $s_k \in \mathrm{R}^1$, $k = 0, \ldots, r$. Assuming the existence of an analytic domain $\mathcal{D}_\omega$ (which in general need not entail satisfaction of the requirements of Nelson's Theorem), Huang, Tarn, and Clark (HTC) were able to derive sufficient conditions for controllability, characterizing the reachable sets $R_t(\psi_o)$ and $R(\psi_o)$ in terms of the three Lie algebras

$$\begin{aligned} \mathcal{A} &= \{\hat{H}_0, \hat{H}_1, ..., \hat{H}_r\}_{\mathrm{LA}} \, , \\ \mathcal{B} &= \{\hat{H}_1, \hat{H}_2, ..., \hat{H}_r\}_{\mathrm{LA}} \, , \\ \mathcal{C} &= \{\mathrm{ad}^j_{\hat{H}_0}\hat{H}_i | i = 1, ..., r; j = 0, 1, ...\}_{\mathrm{LA}} \, , \end{aligned} \tag{9}$$

where $\mathrm{ad}^j_X Y = [X, \mathrm{ad}^{j-1}_X Y]$, $j \geq 1$, with $\mathrm{ad}^0_X Y = Y$. Of special significance are the dimensionalities of the tangent subspaces $\mathcal{A}(\phi)$, $\mathcal{B}(\phi)$, and $\mathcal{C}(\phi)$ of $\mathrm{M} \cap \mathcal{D}_\omega$ at $\phi \in \mathrm{M} \cap \mathcal{D}_\omega$ defined by the vector fields associated with these Lie algebras.

The following key result appears as a corollary of the main theorem (the so-called HTC theorem [16]) proven by Huang, Tarn, and Clark [3]. The statement and application of the corollary are less cumbersome than those of the theorem itself.

HTC Corollary 1. Let $\mathcal{C} = \{\mathrm{ad}^j_{\hat{H}_0}\hat{H}_i | i = 1, ..., r; j = 0, 1, ...\}_{\mathrm{LA}}$ be the ideal in the Lie Algebra $\mathcal{A} = \{\hat{H}_0, \hat{H}_1, ..., \hat{H}_r\}_{\mathrm{LA}}$ generated by $\hat{H}_1, ..., \hat{H}_r$. The system (8), with piecewise-constant controls, is *strongly analytically controllable* on M provided that (i) $[\mathcal{C}, \mathcal{B}] \subset \mathcal{B}$ and (ii) $\dim \mathcal{C}(\phi) = d < \infty$ for all $\phi \in \mathrm{M} \cap \mathcal{D}_\omega$.

Spelled out, condition (i) of this corollary means that $X \in \mathcal{C}$, $Y \in \mathcal{B}$ implies $[X, Y] \in \mathcal{B}$; in other words, the Lie algebra $\mathcal{B}$ must be an ideal in $\mathcal{C}$. Condition (ii) requires that the tangent space associated with $\mathcal{C}$ at ϕ have constant, finite dimension d for all points ϕ on the intersection of $\mathcal{D}_\omega$ and M. If these conditions are met, we can always control the system so that the state $\psi(t)$, starting at any point $\psi_o \in \mathrm{M} \cap \mathcal{D}_\omega$, arrives arbitrarily close to any desired point in the (finite-dimensional) manifold M after any desired time interval t.

Considering that it is applicable to quantum systems having a state space of infinite dimension, this controllability result looks rather positive. However, within the confines of Nelson's Theorem and this ensuing result, not all we might desire is within our grasp. Intuitively, we realize that an infinite sequence of switchings among the piecewise-constant controls would be needed to reach an arbitrary goal on the unit sphere in Hilbert space – a patently unattainable requirement. This hard fact is formalized in the following statement.

HTC Corollary 2 (No-Go Theorem). Suppose the set $\{\hat{H}_0, \hat{H}_1, ..., \hat{H}_r\}$ generates a d-dimensional Lie algebra $\mathcal{A}$ which admits an analytic domain $\mathcal{D}_\omega$. Then the quantum system (8) is *not* analytically controllable on the *full* unit sphere $S_\mathcal{H}$ if d is finite.

It is illuminating to consider some simple examples that satisfy the conditions of HTC Corollary 1 and hence manifest analytic controllability.

Example 1 (Free Particle). In this simplest of examples, the Hamiltonian is just $H_0 = p^2/2m$. Going to skew-Hermitian operators, we have $\hat{H}_0 = -ip^2/2m$ and take $\hat{H}_1 = -ip$ and $\hat{H}_2 = -ix$. Referring to definitions (9), we see that $\mathcal{B}$ is the so-called Heisenberg algebra [40], which is known to be an ideal in the Lie algebra of all observables that are at most of degree 2 in p and x and hence is an ideal in $\mathcal{A}$. Moreover, $\mathcal{B}$ is also an ideal in $\mathcal{C}$, satisfying the key condition of HTC Corollary 1. The eigenstates of p^2 are of course the plane waves when viewed in the position representation, while the operator x generates a shift of momentum value from k to $k+\eta$ via the unitary transformation $S(\eta) = e^{i\eta x}$ (with η a real parameter). An analytic domain can be constructed from superpositions of plane-wave states over finite ranges of momenta.

Example 2 (Rigid Rotor). The Hamiltonian without control is simply $H_0 = \mathbf{J}^2/2I$, where I is the moment of inertia and the components J_x, J_y, and J_z of the (purely orbital) angular momentum $\mathbf{J}$ obey the usual commutation relations

$$[J_x, J_y] = iJ_z\,, \quad [J_y, J_z] = iJ_x\,, \quad [J_z, J_x] = iJ_y\,. \tag{10}$$

Taking $\hat{H}_1 = -iJ_x$, $\hat{H}_2 = -iJ_y$, and $\hat{H}_3 = -iJ_z$, the Lie algebras $\mathcal{A}$, $\mathcal{B}$, and $\mathcal{C}$ are seen to coincide, $\mathbf{J}^2$ being the Casimir operator of the algebra $\mathcal{A}$. So analytic controllability follows (assuming the existence of an analytic domain). The energy levels $E(J, M_J)$ of the system without controls are discrete and are $(2J+1)-$fold degenerate in the magnetic quantum number M_J. Here $J(J+1)$ and M_J are respectively the eigenvalues of $\mathbf{J}^2$ and (say) J_z, with J a non-negative integer and $M_J = -J, \ldots, +J$. The eigenfunctions of H_0 and $\hat{H}_0$ in the position representation are the spherical harmonics $Y_J^{M_J}(\theta, \varphi)$.

We encounter here a peculiar situation: although analytic controllability strictly holds, it is not possible to change the angular momentum quantum number J of the system with the available controls. The system evolves on a $(2J + 1)$-dimensional manifold and it is only possible to change the value of the magnetic quantum number M_J (via J_x or J_y). This example illustrates a general property of quantum control systems: If the autonomous (or "free") evolution is driven by a Casimir invariant (i.e., if H_0 commutes with the controls H_i), the system state will always remain in the subspace of a particular eigenvalue of H_0 – even if the technical requirements for controllability (on the manifold M!) are met.

Example 3 (Harmonic Oscillator). The HTC theorem embraces a physical example of prime importance for physical, chemical, and engineering applications: namely the simple, one-dimensional harmonic oscillator of mass m with coupling to independent external classical fields through its position and momentum observables. With $m = 1$ (and $\hbar = 1$) this problem is mapped into control system (8) through the identifications

$$\hat{H}_0 = -iK_3\,, \qquad \hat{H}_1 = K_+ - K_-\,, \qquad \hat{H}_2 = i(K_+ + K_-)\,, \tag{11}$$

where

$$K_\pm = \pm 2^{-1/2}(\partial_x \mp x)\,, \qquad K_3 = (-\partial_x^2 + x^2)/2\,, \tag{12}$$

while the control functions $u_1(t)$ and $u_2(t)$ are interpreted as the external classical fields (assumed piecewise constant in t). Obviously, the operators K_+ and K_- create and destroy harmonic excitations (phonons). The Lie bracket among the $\hat{H}_i$ is determined via

$$[K_3, K_\pm] = \pm K_\pm\,, \qquad [K_+, K_-] = -I\,, \tag{13}$$

where I is the identity operator.

Our visceral expectation is that the dynamical effect of the drift operator $\hat{H}_0 = -iK_3$ can be cancelled by that of some input that dominates $\mathcal{B}$, assuring strong analytic controllability. This judgment is reflected in the geometric analysis of the problem: It is well known that there is a common dense invariant analytic domain $\mathcal{D}_\omega$ for the operators (11); adopting the position representation, this domain is spanned by analytic functions which are just the

Hermite polynomials, denoted $\eta_n(x)$, $n = 0, 1, 2, ..., \infty$. On the other hand, the Lie algebras $\mathcal{B}$ and $\mathcal{C}$ are readily seen to coincide, so that the required property $[\mathcal{C}, \mathcal{B}] \subset \mathcal{B}$ ensues trivially. From

$$\begin{aligned} K_+\eta_n &= (n+1)^{1/2}\eta_{n+1}\,, \qquad K_-\eta_n = n^{1/2}\eta_{n-1}\,, \\ K_3\eta_n &= (n+\frac{1}{2})\eta_n\,, \qquad I\eta_n = \eta_n\,, \end{aligned} \tag{14}$$

it follows that $\dim \mathcal{A}(\phi) = \dim \mathcal{B}(\phi) = \dim \mathcal{C}(\phi) = d = 3$ for all $\phi \in \mathcal{D}_\omega$, and indeed $\dim I(\mathcal{C}, \xi) = 3$ for all $\xi \in S_{\mathcal{H}} \cap \mathcal{D}_\omega$, where $I(\mathcal{C}, \xi)$ is the maximal integral manifold of $\mathcal{C}$ passing through ξ.

Corollary 1 of the HTC Theorem clearly applies, and we may conclude that (i) the reachable set of ψ_o in $S_{\mathcal{H}} \cap \mathcal{D}_\omega$ is given by $I(\mathcal{C}, \psi_o) = I(\mathcal{B}, \psi_o)$ for $\psi_o = \psi(x; t = 0) \in \mathrm{span}\{\phi_n(x), n = 0, 1, 2, ...\}$, and (ii) with M equal to the closure of $I(\mathcal{B}, \psi_o)$, the system is strongly analytically controllable on M.

It must be emphasized that we have appealed to Nelson's Theorem as a vehicle for rigorizing the exponential formula (2) as a globally valid expression for the time-development operator U. Acceptance of the conditions of that theorem necessarily restricts the manifold M to finite dimension. It is by no means ruled out that stronger controllability results can somehow be derived outside the framework of Nelson's Theorem. In that sense our strategy for handling the domain problems arising for unbounded operators may be regarded as "overkill," especially if one believes that a finite-dimensional description is sufficient for practical purposes. We hasten to add that the analysis reviewed above subsumes the case of a finite-dimensional state space considered later by other authors.

It is nevertheless apparent that complete controllability will not always be attainable, whether for mathematical or practical reasons. (For example, NP-complete problems may be encountered in attempts to construct optimal controls in systems of any complexity, even in the finite-level or finite-dimensional context [41].) Therefore it is sensible to develop "tailored controllability concepts" [44] suitable for technologically important problems, including control on specified subspaces or manifolds and various forms of approximate control.

We call attention especially to a recent effort [28] that lays a basis for quantum computation over continuous variables. The notion of universal quantum computation over continuous variables is certainly precarious: an infinite number of parameters is required to specify an arbitrary transformation over even a single continuous variable (e.g. position x or momentum p); one has no assurance that an arbitrary unitary transformation can be approximated by any finite number of continuous quantum operations; and the susceptibility to noise and decoherence is daunting. Even so, taking a pragmatic approach and implicitly assuming that the domain problems raised above can be sorted out satisfactorily, Lloyd and Braunstein show that it makes sense to define the notion of quantum computation over continuous variables for *subclasses* of unitary transformations, in particular, those that correspond, through exponentiation *à la* Eq. (2), to Hamiltonians H_i that are polynomials of the operators associated with the selected continuous variables. A set of continuous quantum operations is considered universal with respect to the given subclass of transformations provided that a finite number of applications of the operations serves to bring one arbitrarily close to an arbitrary transformation of the subclass. Appealing to the same geometric construction elaborated upon in Sec. 2, it is straightforward to demonstrate that repeated commutations among the "Hamiltonians" $\pm x$, $\pm p$, $H = (x^2 + p^2)/2$, and $\pm S = \pm(xp + px)/2$ provide for the construction of any Hamiltonian quadratic in x and p (and of no Hamiltonian of higher order). (Note that this intermediate result is of interest in connection with Examples 1 and 3 presented above.) Introduction of at least one "nonlinear" operation is needed to build higher-order Hamiltonians; Lloyd and Braunstein find that the Kerr Hamiltonian $H^2 = (x^2 + p^2)^2$ suffices for this purpose (though any higher-order Hamiltonian will work). Adding this extra ingredient to the mix, repeated commutation allows one to create Hamiltonians that are arbitrary Hermitian polynomials of any finite orders in x and p. It is asserted that the number of operations increases as a small polynomial in the order of the polynomial that is to be formed. Extension to the case of many variables $\{x_i, p_i\}$ is achieved through the inclusion of a set of interaction Hamiltonians $\pm B_{ij} = \pm(p_i x_j - x_i p_j)$. The authors proceed to address issues of electro-optical implementation based on beam splitters, phase shifters, squeezers, Kerr-effect fibers, and optical cavities, as well as the problem of error correction as a remedy for noise. This effort represents seminal formal progress on the interface of quantum control and quantum computation.

IV. IMPLICATIONS FOR QUANTUM MANY-BODY THEORY

For the many-body theorist, the exciting new developments in quantum control and quantum computation offer opportunities to contribute and opportunities to benefit.

A. Quantum Control

Laser control of matter requires a subtle cooperation between the light and matter systems to produce the precise interference of quantum pathways that is essential to achieving the desired outcome of an experiment or technological application. Intuition is likely to be insufficient for the determination of a proper laser signal. This realization has led to the introduction of systematic theoretical tools for the design of control fields.

One needs to distinguish between *open-loop* and *closed-loop* control scenarios. In closed-loop control, information is extracted from the output in real time to guide the design of the control field; whereas in open-loop control one merely imposes a pre-determined field. The former is evidently problematic in the case of a quantum system, since collapse of the wave packet ensues if a measurement extracts classical information. For more discussion of this point see Lloyd [25], who envisions an alternative and potentially more powerful closed-loop scenario (*quantum feedback control*) in which quantum rather than classical information is obtained and coherence is preserved.

We note, incidentally, that the destructive effect of classical measurement is actually innocuous in "closed-loop" *learning control*, proposed by Judson and Rabitz [12] and recently put into practice by Bardeen *et al.* [49] and Assion *et al.* [50]. In this hybrid experimental/theoretical scheme, the system to be controlled "teaches" a computer-programmable laser pulse shaper to find the optimal control field. A rapid sequence of experiments is performed, in each of which the response of the sample is probed and fed into a learning algorithm that computes incremental corrections to the control field. Once the optimal field is determined, it can be applied to a "fresh" system that is not subsequently probed.

Theoretical methods for implementing open-loop control include path-planning on unitary groups [46–48], optimal control [9,10], and inverse control [11]. The first of these, intended specifically for finite-level systems, is a geometric approach in which controls yielding a target time-development operator (and hence a target state) are determined explicitly by exploiting the algebraic structure of unitary groups under a variety of constraints on the controls. In the second method, the variational principle is applied to achieve the "best possible" outcome subject to obedience of the Schrödinger equation and to certain practical constraints on the control fields. In the third, one seeks a control that produces a prescribed track for the expectation value of some system observable; this approach has the advantage that one can solve for the requisite control field upon invoking the Heisenberg equation of motion for the expectation value [4]. All these methods demand, in principle, complete knowledge of the autonomous system Hamiltonian and the field couplings (e.g. transition dipole moments). All require accurate solution of the Schrödinger equation in one form or another. Implementation of the optimal control approach requires solution of a two-point boundary value problem involving integration of Schrödinger equations forward and backward in time. Implementation of inverse control requires solution of the Schrödinger equation with the control present, in order to evaluate certain expectation values entering the solution for the control field. To date, these methods have only been applied to the simplest of model systems, or the simplest of molecules. Beyond these cases, the computational dimensions become formidable, and the full arsenal of microscopic quantum many-body theory will be needed to make significant advances. The involvement of computational many-body theorists would be crucial to such an effort. One of the rewards of the inevitable iteration process of calculation and comparison with experiment (notably in the enlarged context of inverse control) would be an enhanced understanding of the system Hamiltonian (e.g. in the form of electronic energy surfaces) as well as the couplings to the external fields.

In similar spirit, the "closed-loop" learning-control scheme exploits the fact that the system "knows" its own Hamiltonian; the system is made to "teach" the necessary aspects of the autonomous Hamiltonian and field couplings to the laser (and indirectly the experimenter).

B. Quantum Computation

The dimension of the space of wave functions of a quantum system grows exponentially with the particle number, presenting an exponential barrier to solution by classical computers. Two decades ago Feynman [20] argued that quantum computers, which by definition can follow many alternative computational paths simultaneously, should be able to overcome this impasse. He further speculated that there may exist quantum computers which can serve as universal simulators of quantum systems. It has recently been argued [51] that Feynman was correct on the second as well as the first count, and that quantum computation will permit solution of many-body problems hitherto regarded as intractable (e.g. macromolecules, heavy nuclei, hadron structure based on QCD). Procedures have been outlined for efficient simulation of the time evolution of Fermi systems (which suffer from the notorious sign problem when simulated on a classical computer) [52], and for exponential speed-up in the determination of eigenvalues and eigenvectors (relative to classical computation) [53]. However, the conditions under which the promise of quantum computation can be realized for strongly interacting many-body systems remains to be established in practical detail [54]. In particular, one must consider that the algorithm offered in Ref. 51 requires an initial guess for the wave function whose overlap with the exact ground state does not become exponentially small with increasing particle number. It should be fruitful to explore this and other issues raised by quantum computation, from the perspective of many-body theory.

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