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Quantum control of infinite-dimensional many-body systems

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A major challenge to the control of infinite-dimensional quantum systems is the irreversibility which is often present in the system dynamics. Here we consider systems with discrete-spectrum Hamiltonians operating over a Schwartz space domain and show that by utilizing the implications of the quantum recurrence theorem this irreversibility may be overcome, in the case of individual states more generally, but also in certain specified cases over larger subsets of the Hilbert space. We discuss briefly the possibility of using these results in the control of infinite-dimensional coupled harmonic oscillators and also draw attention to some of the issues and open questions arising from this and related work.

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I. INTRODUCTION

One of the main goals of control theory in quantum mechanics is to characterize the achievable dynamics of a system in relation to a given set of control fields. While such *reachable sets* are well understood in the case of finite-dimensional systems [1], the same cannot be said about infinite-dimensional systems. Apart from the usual mathematical problems of infinite-dimensional systems, such as unbounded operators and the inequivalence of norms, the main *physical* obstacle is that infinite-dimensional systems generally show some form of *irreversible* dynamics, which means they are not controllable in general; and this causes further problems on a mathematical level because the systems' reachable sets cannot be captured *algebraically* (that is, by looking at short-term dynamics only). A typical way this obstacle manifests itself is in the *drift Hamiltonian*, which is the part of the system interaction which is always present, independent of the applied controls, and which as such can be the cause of irreversible dynamics.

From a physics perspective, the most relevant infinite-dimensional systems are those with position (and potentially spin) degrees of freedom. In this case, it was shown in the seminal work by Braunstein and Lloyd [2] that in the absence of a drift Hamiltonian, any Hamiltonian can effectively be reached by switching between various quadratic Hamiltonians and a single generic higher-order one. Specific simple periodic drift Hamiltonians were also considered. The work in Ref. [2] was put in a rigorous mathematical framework in Ref. [3]. Braunstein's result is very suitable for quantum optics but does not apply to systems with constant many-body interactions. This is, for instance, the case in systems of nanomechanical oscillators [4] and in solid-state systems described by Bose-Hubbard interactions [5]. For these systems, specific examples of quantum control were developed by the authors of Ref. [6] using the Baker-Campbell-Hausdorff formula and extensive numerical analysis, but no general results regarding reachability were given.

Recently, we developed a framework for quantum control of positive definite quadratic Hamiltonians in the presence of drift Hamiltonians [7]. Our analysis made use of the finite-dimensional symplectic representation as well as the quantum recurrence theorem, and gave a general proof of previous numerical observations [8]. Here, we obtain a generalization of this work that only relies on Hamiltonians with discrete

eigenvalues, using the quantum recurrence theorem. Essentially, such Hamiltonians naturally occur when the relevant system has only bound states, so this case captures almost all relevant control applications (see also Ref. [9] for a discussion of such Hamiltonians, relevant to the cases discussed here).

Finally, we apply our results to coupled oscillator systems and show that the methods developed here allow us to substantially extend recent results on indirect control [7,10] to the infinite-dimensional case.

II. SETUP

For simplicity we will ignore any spin degrees of freedom and consider wavefunctions in one spatial dimension only (the generalization is straightforward). Much previous work in infinite-dimensional control has been done treating closed-loop systems, where system feedback is utilized in implementing the control (see, for instance, Ref. [11] and references therein). Here, however, we are focusing on open-loop controls, which do not employ feedback and thereby avoid any possible complications arising from measurement of the quantum system. We consider the Hilbert space \mathcal{H} of square-integrable wavefunctions [i.e., the space $L^2(\mathbb{R})$] and a finite set of self-adjoint operators $\tilde{\mathcal{A}} = \{\tilde{H}_1, \tilde{H}_2, \dots, \tilde{H}_K\}$, which are assumed to be polynomials in position and momentum. The set $\tilde{\mathcal{A}}$ describes the *directly implementable Hamiltonians*, i.e., the set of available Hamiltonians between which the experimentalist may switch at will. Hence, a control sequence consists of a list of times (t_1, t_2, \dots, t_n) , $t_j \geq 0$, and another of Hamiltonian choices (k_1, k_2, \dots, k_n) , $1 \leq k_j \leq K$, such that from time 0 to t_1 , the system evolves under \tilde{H}_{k_1} , from t_1 to t_2 under \tilde{H}_{k_2} and so on. Note that the set $\tilde{\mathcal{A}}$ may also describe systems with a drift Hamiltonian \tilde{H}_0 , e.g., by writing $\tilde{H}_j = \tilde{H}_0 + H'_j$, and that continuous control sequences can be described in a manner similar to the piecewise constant case discussed here. Assuming use of natural units throughout, so that $\hbar = 1$, we shall further simplify notation hereafter by defining the set of skew-adjoint operators $\mathcal{A} = \{H_1, H_2, \dots, H_K\}$, where $H_j = -i\tilde{H}_j$ for each $j = 1, \dots, K$.

As for domains, we follow Ref. [3] and consider the Schwarz space

$$\mathcal{H}_s = \{\psi \in \mathcal{H} \mid \sup_{k,l \geq 0} \|p^k q^l \psi\| < \infty\}, \quad (1)$$

where $\|\cdot\|$ is the Hilbert space norm and p and q are the momentum and position operators, respectively. This is a dense subspace of \mathcal{H} , on which $\bar{\mathcal{A}}$ is defined. We will use the following theorems [3]:

$$\lim_{n \rightarrow \infty} (e^{H_k \frac{t}{n}} e^{H_\ell \frac{t}{n}})^n \psi = e^{(H_k + H_\ell)t} \psi, \quad (2)$$

$$\lim_{n \rightarrow \infty} (e^{-H_k \frac{t}{n}} e^{-H_\ell \frac{t}{n}} e^{H_k \frac{t}{n}} e^{H_\ell \frac{t}{n}})^n \psi = e^{[H_k, H_\ell]t^2} \psi, \quad (3)$$

where $H_k, H_\ell \in \mathcal{A}$, and $\psi \in \mathcal{H}_S$. Note that to utilize Eq. (3) we need to be able to employ $-H_k$ and $-H_\ell$ for $H_k, H_\ell \in \mathcal{A}$. How to do this when $-H_k, -H_\ell \notin \mathcal{A}$ is the central problem addressed in this paper.

The reachable set \mathcal{R} from an initial state $\psi_0 \in \mathcal{H}_S$ is given by the states for which there exists a control such that they become solutions to the Schrödinger equation with initial condition ψ_0 , i.e.,

$$\mathcal{R}(\psi_0) = \left\{ \left[\prod_{j=1}^n (e^{H_j t_j}) \right] \psi_0 \mid H_j \in \mathcal{A}, t_j \geq 0, n \in \mathbb{N} \right\}. \quad (4)$$

Similarly, we have the reachable set of unitaries, \mathcal{U} , given by

$$\mathcal{U} = \left\{ \prod_{j=1}^n e^{H_j t_j} \mid H_j \in \mathcal{A}, t_j \geq 0, n \in \mathbb{N} \right\}. \quad (5)$$

We define the dynamical Lie algebra $\mathfrak{l}_s \equiv \langle \mathcal{A} \rangle_{[-, \cdot]}$ of the system as the real Lie algebra generated by \mathcal{A} , i.e., the set of operators one obtains from \mathcal{A} through real linear combinations and commutators. Defining $\mathfrak{l}_s / (-i) \equiv \{l / (-i) \mid l \in \mathfrak{l}_s\}$, note that any element $\tilde{H} \in \mathfrak{l}_s / (-i)$ is a polynomial in position and momentum and self-adjoint with domain $D(\tilde{H}) \supset \mathcal{H}_S$.

III. CONTROLLABILITY

In this section we will provide some theorems that allow us to characterize the controllability of infinite-dimensional systems through *reachable sets*. First we use the quantum recurrence theorem to show that if each element in \mathcal{A} has a discrete spectrum, then irreversibility can be overcome and with regard to the reachable set from a specific starting state ψ_0 we have that $\bar{\mathcal{R}}(\psi_0) \supset e^{\mathfrak{l}_s} \psi_0$, where $\bar{\mathcal{R}}$ denotes the norm closure of \mathcal{R} .¹ This result is analogous to the finite-dimensional characterization [1]. Because recurrence times are usually state-dependent, such point-wise characterizations can only be extended to larger sets using further structure. To this end, we show that for any *compact* set in Schwarz space the closure of the set of reachable unitaries contains $e^{\mathfrak{l}_s}$. In practice this implies that unitaries can be implemented arbitrarily well on any finite collection of states. Finally, motivated by physics, we consider the case that each element in \mathcal{A} has a spectrum of energy eigenvalues that is bounded below and has no

accumulation points.² We show in that case that any set of states with an overall bound on the *energy expectation values* with respect to \mathcal{A} contains $e^{\mathfrak{l}_s}$ in the closure of its reachable set of unitaries.

A key result employed here is the quantum recurrence theorem [12,13]. So long as our system is evolving under the influence of a constant Hamiltonian that has a discrete spectrum of energy eigenvalues, then the theorem tells us that if our system is in the state $\psi(T_k)$ at time T_k , then as the system evolves in time, there will for any $\tau, \delta > 0$ occur a time $T_l > T_k + \tau$ such that $\|\psi(T_k) - \psi(T_l)\| < \delta$ (where $\psi(T_l)$ is the state at time T_l). That is, if one waits long enough from an initial time T_k the system will always return arbitrarily close to the state $\psi(T_k)$ in which it was at time T_k . Note as well that by the theory of almost-periodic functions [14] the recurrence implied by the theorem in fact represents an *infinite* sequence of such recurrences for any δ .

Theorem 1. If each element in \mathcal{A} has a discrete spectrum, then $e^{\mathfrak{l}_s} \psi_0 \subset \bar{\mathcal{R}}(\psi_0)$.

Proof. For any $H_k \in \mathcal{A}$, we have $e^{H_k t_k} \psi_0 \in \mathcal{R}(\psi_0) \subset \bar{\mathcal{R}}(\psi_0)$ for any $t_k \geq 0$, by our definition of $\mathcal{R}(\psi_0)$ above. Consider now the case of $e^{-H_k t_k} \psi_0$ for $H_k \in \mathcal{A}$, $t_k > 0$. Now, because H_k has a discrete spectrum we may invoke the quantum recurrence theorem to show that for any $\delta > 0$ there exists a $t_{k^*} \geq 0$ ($\Rightarrow t_k + t_{k^*} > 0$) such that $\|\psi_0 - e^{H_k t_k} e^{H_k t_{k^*}} \psi_0\| = \|\psi_0 - e^{H_k(t_k + t_{k^*})} \psi_0\| < \delta$. By the unitarity of the exponential operators, this implies equivalently that $\|e^{-H_k t_k} \psi_0 - e^{H_k t_{k^*}} \psi_0\| < \delta$. As $e^{H_k t_{k^*}} \psi_0 \in \mathcal{R}(\psi_0)$ for $t_{k^*} > 0$, it follows that $e^{-H_k t_k} \psi_0 \in \bar{\mathcal{R}}(\psi_0)$. Now, for $H_k, H_l \in \mathcal{A}$, $t_{k,l} \in \mathbb{R}$, Eqs. (2) and (3) allow us to approximate $e^{(H_k + H_l)t_{k,l}} \psi_0$ and $e^{[H_k, H_l]t_{k,l}} \psi_0$, respectively, with an arbitrary degree of accuracy. It follows that $e^{(H_k + H_l)t_{k,l}} \psi_0, e^{[H_k, H_l]t_{k,l}} \psi_0 \in \bar{\mathcal{R}}(\psi_0)$. Combining the above we have that $e^{\mathfrak{l}_s} \psi_0 \subset \bar{\mathcal{R}}(\psi_0)$. ■

The result of Theorem 1 is applicable to any $\psi_0 \in \mathcal{H}_S$, but in general only to such ψ_0 considered individually. In the context of quantum computing this is especially problematic, first because we would like in general to implement unitary operations not just on individual states but across subsets of the Hilbert space, and second because we may not in any case be able to possess perfect information about the initial state. The ability to perform a unitary operation reliably over a set of states close to the one of interest thus provides a stability condition for the controllability of the system. In the following two theorems we extend the result to larger subsets of \mathcal{H}_S . In both cases the result depends on the details of the proof of the quantum recurrence theorem, outlined below. The point is that recurrence times usually depend on the state, making the control sequence state-dependent in turn. Under the extra condition of compactness or finite energy expectation, however, state-independent recurrence times, and thus state-independent control sequences, may be found.

As a solution to the Schrödinger equation at time T_k , with a constant discrete-spectrum Hamiltonian, the state $\psi(T_k)$ may be expanded as the infinite sum $\psi(T_k) = \sum_{n=0}^{\infty} c_n e^{-iE_n T_k} \phi_n$,

¹Note that in infinite dimensions the closures of \mathcal{R} and \mathcal{U} contain unphysical elements. This does not pose a problem here as we are only interested in physical elements that can be approximated arbitrarily closely with elements of \mathcal{R} and \mathcal{U} .

²In the context of this paper, this lack of accumulation points is equivalent to there being no finite interval of \mathbb{R} that contains an infinite number of energy eigenvalues.

where the c_n are complex coefficients depending on $\psi(T_k)$ (with $\sum_{n=0}^{\infty} |c_n|^2 = 1$), and the ϕ_n are orthogonal eigenstates corresponding to the Hamiltonian's discrete energy eigenvalues E_n . Assuming the Hamiltonian remains constant, a state $\psi(T_l)$ at time $T_l > T_k$ may be similarly expanded as $\psi(T_l) = \sum_{n=0}^{\infty} c_n e^{-iE_n T_l} \phi_n$, and then it follows that

$$\|\psi(T_k) - \psi(T_l)\|^2 = 2 \sum_{n=0}^{\infty} |c_n|^2 [1 - \cos(E_n \tilde{T})],$$

where $\tilde{T} = T_l - T_k$. Now, because $\sum_{n=0}^{\infty} |c_n|^2 = 1$, it is possible for any $\delta > 0$ to choose an $N \in \mathbb{N}$ such that

$$\sum_{n=N+1}^{\infty} |c_n|^2 < \frac{\delta^2}{8}. \tag{6}$$

Furthermore, by the theory of almost-periodic functions [14] it will always be possible to find a value of \tilde{T} (or indeed an infinite sequence of such values) such that for any $\delta > 0$

$$\sum_{n=0}^N [1 - \cos(E_n \tilde{T})] < \frac{\delta^2}{4}. \tag{7}$$

Combining these facts, with N suitably chosen in Eq. (6) and \tilde{T} suitably chosen in Eq. (7), gives us

$$\begin{aligned} \|\psi(T_k) - \psi(T_l)\|^2 &= 2 \sum_{n=0}^{\infty} |c_n|^2 [1 - \cos(E_n \tilde{T})] \\ &\leq 2 \sum_{n=0}^N [1 - \cos(E_n \tilde{T})] + 4 \sum_{n=N+1}^{\infty} |c_n|^2 \\ &< \frac{\delta^2}{2} + \frac{\delta^2}{2} = \delta^2, \end{aligned}$$

from which it follows that $\|\psi(T_k) - \psi(T_l)\| < \delta$, as desired. Note that in Eq. (7) the choice of \tilde{T} depends only on the E_n , which are in turn dependent only on the Hamiltonian; i.e., the choice of \tilde{T} is independent of the particular system state vectors under consideration.

Theorem 2. For unitaries $e^{H_j t_j}$ ($H_j \in \mathcal{A}, t_j \geq 0$) operating on any compact set $X \subset \mathcal{H}_S, e^{t_s} \subset \bar{\mathcal{U}}$.

Proof. For $H_k \in \mathcal{A}, t_k \geq 0$, we have $e^{H_k t_k} \in \mathcal{U} \subset \bar{\mathcal{U}}$. Now consider the unitary $e^{-H_k t_k}$ for $H_k \in \mathcal{A}, t_k > 0$. Let $\varepsilon > 0$ be given, and let $\mathcal{B} = \{B(\psi) | \psi \in X\}$, where $B(\psi) = \{\phi \in \mathcal{H}_S | \|\phi - \psi\| < \frac{\varepsilon}{3}\}$. This is an open covering of X , so by compactness we may choose a finite subcovering $\tilde{\mathcal{B}} = \{B(\psi_i) | B(\psi_i) \in \mathcal{B}, i = 1, \dots, q\}$. Let $\delta = \frac{\varepsilon}{3}$ in Eqs. (6) and (7) above. For each ψ_i we may choose an $N_i \in \mathbb{N}$ satisfying Eq. (6); let $N = \max\{N_i : i = 1, \dots, q\}$. Having made this choice of N , we may choose a $\tilde{T} = t_k + t_{k^*} > 0$ (with $t_{k^*} \geq 0$) satisfying Eq. (7), where the choice of \tilde{T} depends only on the energy eigenvalues of \tilde{H}_k . With this choice of N and \tilde{T} , it follows that $\|\psi_i - e^{H_k(t_k+t_{k^*})}\psi_i\| < \frac{\varepsilon}{3}$, or equivalently that $\|e^{-H_k t_k}\psi_i - e^{H_k t_{k^*}}\psi_i\| < \frac{\varepsilon}{3}$, for all $\psi_i, i = 1, \dots, q$. Now consider an arbitrary $\psi \in X$. Noting that every such ψ is contained in some $B(\psi_i)$, and using the triangle inequality,

we have that

$$\begin{aligned} &\|e^{-H_k t_k}\psi - e^{H_k t_{k^*}}\psi\| \\ &\leq \|e^{-H_k t_k}\psi - e^{-H_k t_k}\psi_i\| + \|e^{-H_k t_k}\psi_i - e^{H_k t_{k^*}}\psi_i\| \\ &\quad + \|e^{H_k t_{k^*}}\psi_i - e^{H_k t_{k^*}}\psi\| \\ &= \|\psi - \psi_i\| + \|e^{-H_k t_k}\psi_i - e^{H_k t_{k^*}}\psi_i\| + \|\psi_i - \psi\| \\ &< \frac{\varepsilon}{3} + \frac{\varepsilon}{3} + \frac{\varepsilon}{3} = \varepsilon. \end{aligned}$$

Thus, we see that $e^{-H_k t_k} \in \bar{\mathcal{U}}$. Now, noting that neither Eq. (2) nor (3) depend on the system state vector ψ under question, then for $H_k, H_l \in \mathcal{A}$ and $t_{k,l} \in \mathbb{R}$ we will have $e^{(H_k+H_l)t_{k,l}}, e^{[H_k, H_l]t_{k,l}} \in \bar{\mathcal{U}}$, for reasons analogous to those in the proof of Theorem 1. Combining the above we have $e^{t_s} \subset \bar{\mathcal{U}}$. ■

Finally, we consider the case of states with bounded energy expectation value.

Theorem 3. If each element in $\tilde{\mathcal{A}}$ has a discrete spectrum of energy eigenvalues that is bounded below and has no accumulation points, then for any set of states $X \subset \mathcal{H}_S$ with an overall bound on the energy expectation values with respect to $\tilde{\mathcal{A}}, e^{t_s} \subset \bar{\mathcal{U}}$.

Proof. Again, $e^{H_k t_k} \in \mathcal{U} \subset \bar{\mathcal{U}}$ for $H_k \in \mathcal{A}, t_k \geq 0$, but we must consider the case for $e^{-H_k t_k}$ with $H_k \in \mathcal{A}, t_k > 0$. For H_k with energy eigenvalues bounded below, we may organize this set of eigenvalues $\{E_0, E_1, E_2, \dots, E_n, \dots\}$ in ascending order, i.e., such that $E_0 \leq E_1 \leq E_2 \leq \dots \leq E_n \leq \dots$ for all $n \in \mathbb{N}$, where we assume without loss of generality that $E_0 \geq 0$. For an infinite-dimensional system this boundedness of the eigenvalues below, combined with the lack of accumulation points, also gives us that $E_n \rightarrow \infty$ as $n \rightarrow \infty$, while by the bound on the energy expectation value we have $\langle \tilde{H}_k \rangle_{\psi} < M$ for all $\tilde{H}_k \in \tilde{\mathcal{A}}, \psi \in X$, and for some finite $M \in \mathbb{R}, M > 0$. Let $\delta > 0$ be given, and choose finite $N \in \mathbb{N}$ such that $E_{N+1} \geq \frac{8M}{\delta^2}$ (noting that the lack of accumulation points makes such a choice possible). Since $E_{N+1} \leq E_{N+2} \leq \dots$, then (with the c_n being the eigenbasis decomposition coefficients as in the proof of the quantum recurrence theorem above) we have that

$$E_{N+1} \sum_{n=N+1}^{\infty} |c_n|^2 \leq \sum_{n=0}^{\infty} |c_n|^2 E_n < M,$$

from which it follows that $\sum_{n=N+1}^{\infty} |c_n|^2 < \frac{M}{E_{N+1}} \leq \frac{\delta^2}{8}$. Note that although this choice of N satisfies Eq. (6) for every $\psi \in X$, the choice depends only on the energy eigenvalues of \tilde{H}_k . Having thus chosen N , we may then make a choice of $\tilde{T} = t_k + t_{k^*}$ (with $t_{k^*} \geq 0$) satisfying Eq. (7), where the choice of \tilde{T} also depends only on the energy eigenvalues of \tilde{H}_k . With this N and \tilde{T} , it follows that for all $\psi \in X$ we have $\|\psi - e^{H_k(t_k+t_{k^*})}\psi\| < \delta$, or equivalently $\|e^{-H_k t_k}\psi - e^{H_k t_{k^*}}\psi\| < \delta$, and therefore that $e^{-H_k t_k} \in \bar{\mathcal{U}}$. As in the proof of Theorem 2, we will now have $e^{(H_k+H_l)t_{k,l}}, e^{[H_k, H_l]t_{k,l}} \in \bar{\mathcal{U}}$ for $H_k, H_l \in \mathcal{A}$ and $t_{k,l} \in \mathbb{R}$. Combining the above we have $e^{t_s} \subset \bar{\mathcal{U}}$. ■

We remark that the same argument to obtain universal recurrence times was made independently in a different context by Wallace [13]. For a consideration of recurrence in the presence of Hamiltonians with discrete spectra, in the context of proving approximate full controllability in certain finite- and infinite-dimensional systems, see also Ref. [15].

IV. EXAMPLE

As an example, we consider a generalization of Ref. [2], where it was shown that cubic terms can generate polynomials of arbitrary order. We will be brief in this presentation; details may be found at Ref. [10]. Let us look at a system of N coupled harmonic oscillators that are interacting through the Hamiltonian $H = \sum_{i,j} a_{ij} H_{ij}$, $a_{ij} \geq 0$, where the interaction is given by coupled oscillators with spring constant ω in the rotating wave approximation

$$H_{ij} = p_i^2 + q_i^2 + p_j^2 + q_j^2 + \omega(p_i - p_j)^2 + \omega(q_i - q_j)^2, \quad (8)$$

and the coupling strengths a_{ij} determine the geometry of the system. If we denote the local Lie algebra of all skew-adjoint polynomials on one oscillator i by \mathfrak{l}_i , and the Lie algebra of skew-adjoint polynomials on two oscillators i and j by \mathfrak{l}_{ij} , then it follows easily from the canonical commutation relationships that

$$\langle \mathfrak{l}_i, [\mathfrak{l}_i, i H_{ij}]_{[\cdot, \cdot]} \rangle = \mathfrak{l}_{ij}, \quad (9)$$

i.e., \mathfrak{l}_{ij} is the smallest Lie algebra that contains \mathfrak{l}_i and elements of the form $[\mathfrak{l}_i, i H_{ij}]$. This property is known as algebraic propagation [10] and implies that an easy criterion can be used to show that the system algebra \mathfrak{l}_s is the complete one defined by the couplings a_{ij} and the controls. Using the fact that H has a discrete spectrum together with our Theorem 1, we find that a chain of oscillators controlled on one end is fully state controllable.

V. CONCLUSIONS

We have extended the well-known characterizations of reachable sets in finite dimensions to a large and physically relevant class of infinite-dimensional systems. Our result raises many interesting issues. First, while in finite dimensions control sequences can in principle be computed numerically, these algorithms become less and less efficient with higher dimensions. While in some cases, going to infinite dimensions will *simplify* the numerics [8], we expect that most control pulses are *uncomputable* with classical computers. Second, it is a long-standing open problem [16] to obtain useful bounds on *how long* it takes to achieve a reachable operation. While numerical examples in finite dimensions often yield short times in practice, we expect that the worst-case examples in finite dimensions can scale as badly as recurrence times—reaching the lifetime of the universe easily. It would be interesting to see how this changes in infinite dimensions, and we conjecture that by introducing physical constraints—such as finite energy expectations of the target states—one can still find many practical controls (see also Ref. [6]).

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