Coarse-Grained Wavepacket Controllability by Free Evolution and Phase Shifts with Smooth Coordinate Dependance.

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We describe an approach to controlling wavepacket dynamics and a criterion of wavepacket controllability based on discretized properties of the wavepacket's localization on the orbit. The notion of "coarse-grained control" and the coarse-grained description of the controllability in infinite-dimensional Hilbert spaces are introduced and studied using the mathematical apparatus of loop groups. We prove that 2D rotational wavepackets are controllable by only free evolution and phase kicks by AC Stark shift implemented at fractional revivals. This scheme works even if the AC Stark shifts can have only a smooth coordinate dependence, correspondent to the action of a linearly polarized laser field.

I. INTRODUCTION

Facing the problem of controlling a quantum system, it is important to know whether the set of tools at hand – mathematically, the set of different Hamiltonians one can apply to the system – is sufficient to implement all desired transformations. With this kind of information, one can either look for intuitive schemes to implement the needed transformation [1, 2], or rely on numerical or experimental optimal control algorithms [3]. If, however, the set of control knobs at hand is proven to be insufficient, one can analyze why it is so and then efficiently search for additional control tools.

Controllability of a quantum system implies the ability to generate any unitary transformation, and hence any state to state transformation, with a given set of control knobs.

Here controllability also implies that any such transformation can be generated in a certain time T_f that does not exceed some boundary value T_0; for discussion of different definitions of controllability see, e.g., [4].

Geometric approach to controllability has been very successful for finite-dimensional Hilbert spaces, i.e. in analyzing the controllability of a system where the evolution is confined to a finite, pre-determined set of levels. It has been used in the areas of atomic and molecular control (see [2], [4]-[8]), as well as in the field of quantum computation ([9]-[12]). The following result is used most commonly: one can generate any unitary transformation in an N-level system, applying the set of time-independent Hamiltonians H_0, ... H_k, if the Lie algebra generated by these Hamiltonians – the space of linear combinations of $H_0, ..H_k$ and their iterated commutators – is of real dimension N^2 [8, 13].

In the physical examples, H_0 often stands for the unperturbed hamiltonian of the system and $H_1, ..., H_k$ include different types of perturbations one can switch on and off, one at a time, for intervals of time that can be arbitrarily short. In the context of atomic and molecular control $H_1, ..., H_k$ are usually meant to be implemented by switching on and off laser pulses of various spectra, intensity, and polarization. It is important to keep in mind that the ability to apply $H_1, ..., H_k$ over arbitrary time intervals implies arbitrarily flexible shaping of the external fields (laser pulses) that provide the perturbations. As a rule, for a finite number of levels two non-commuting Hamiltonians are sufficient to generate Lie algebra of real dimension N^2 [10].

Thus, for a finite-level atomic or molecular system, knowing the transition matrix elements for laser pulses at hand, one has a fairly straightforward way of telling whether the system is controllable or not.

However, most real systems are infinite-dimensional. Simple yet fundamental model involving infinite number of levels is a bound motion of a wavepacket in a system with discrete infinite-dimensional spectrum, where any superposition of states can be excited. Obvious examples include harmonic oscillator, Rydberg atom, or a rotor. A wavepacket is both one of the most basic quantum-mechanical concepts and one of the typical control entities. Experiments attempting to utilize and control wavepacket dynamics span such areas as photochemistry, intense laser-matter interaction and quantum computation (see, e.g., [1, 2, 14–16]).

Unfortunately, for infinite-dimensional systems, very little is known regarding controllability. Application of geometric methods to describe infinite-dimensional control is difficult; the theory of infinite-dimensional Lie groups is not yet well developed. In general, the prediction is negative in the sense that, using piecewise-constant controls, global controllability cannot be achieved with a finite number of operations [17]. Controllability is achieved over some part of the Hilbert space, if the initial condition and the dynamics are restricted to a finite-dimensional manifold (thus, the Lie algebra generated by all Hamiltonians at hand is finite-dimensional), see [7, 8, 17]. Only in a few cases dealing with special types of controlling Hamiltonians one can achieve control over infinite-dimensional *state* of the system [7, 18] (rather than the whole evolution matrix), or over an infinite-dimensional subset of all the possible evolution matrices [19].

Moreover, if the number of levels involved is finite but very large, then the general picture also looks rather pessimistic. In order to explore all the dimensions needed for controllability, as the dimension of the corresponding Lie algebra scales as N^2, one has to scale accordingly the number of control knobs: the number of piece-wise constant non-commuting Hamiltonians, or the number of different laser frequencies with controlled amplitudes and phases, etc. Alternatively, one has to apply sequences of interactions of growing length. Note that many interesting control experiments [16] are done in the non-perturbative regime, where the laser field couples and modifies many eigenstates, so that it is rarely possible to single out a small isolated subsystem controlled by the field.

We suggest and study one possible way to deal with these difficulties. Dealing with a wavepacket, one is mostly interested in the features of its localization. It is the degree and the region of wavepacket localization in the phase space that are reasonable objectives of control. In the spirit of a bulk of experiments on femtosecond control, we reformulate the question of controllability following the idea that *only coarse-grained information on the wavepacket structure and localization* is of interest.

We focus on wavepackets which evolve in a system with infinite-dimensional spectrum with energies depending quadratically on the quantum number, such as a rigid rotor. Given a desired degree of wavepacket localization, we use the wavepacket spreading and the so-called wavepacket revivals [20] to map complex infinite-dimensional evolution onto that of a few replicas of the same wavepacket, evenly distributed along the generalized angle variable on the corresponding classical orbit.

The number of such replicas is determined by the amount of information one wants to track. Their evolution and controllability is described using the apparatus of loop groups. The latter allows us to make conclusions about the conditions of controllability in an infinite-dimensional system.

The most important aspect of our coarse-grained approach and the loop groups-based analysis is that they allow us to deal with infinite-dimensional system without specifying (or restricting) the number of levels involved in the dynamics. The coarse-grained approach allows us to introduce a finite-dimensional control basis where each basis vector is a wavepacket and is, in principle, infinite-dimensional – but is addressed as a whole.

In our control approach, the wavepackets are controlled by coordinate-dependent phase-shifts applied to the basis wavepackets. These phase-shifts can be implemented via nonresonant AC Stark shift induced by short laser pulses. As a result of such short "kicks", the Stark shift changes the phase of the wavefunction in a coordinate-dependent way, mixing *all* eigenstates.

The rest of the paper is outlined as follows. First, we introduce a model of a 2D rotor and describe the wavepacket dynamics on the spreading-revival timescale [20]. Using arguments about physical purposes of the control, we introduce the concept of the coarse-grained control and the control method based on applying coordinate-dependent phase kicks to the wavepacket. The phase kicks are applied at the wavepacket's fractional revivals. We introduce the mathematical description of the control procedure using the apparatus of loop groups and show that rotational wavepackets are controllable by the phase shifts which smoothly depend on the coordinate. The analysis does not restrict the number of levels involved in the dynamics. Then, we discuss the conditions for limiting the amount of noise in the generated unitary transforms and possible generalization of our method to an arbitrary 1D wavepacket with weakly nonlinear spectrum. The last Section presents our conclusions.

II. PHYSICAL REASONING AND THE CONTROL MODEL.

As a main example, we consider the control of a 2D rigid rotor confined to a plane. This system allows for the easiest explanation of our ideas; generalization to other systems with nonlinear spectrum will be discussed in the Section V.

The 2D rotor's spectrum and eigenstates are given by

$$E_M = BM^2, \quad M = -\infty ... \infty \tag{1}$$

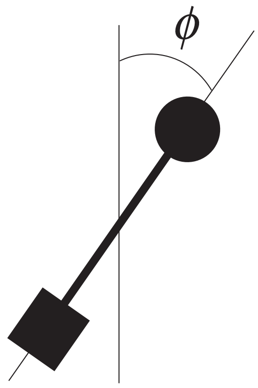

FIG. 1: Schematic view of a planar rotor

$$\psi_M(\phi) = \frac{1}{\sqrt{2\pi}} e^{iM\phi} \tag{2}$$

where M is the quantum number of the planar rotational eigenstate, ϕ is the orientation angle of the rotor (Fig.1).

Fig.2(a) shows the so-called quantum carpet [21] – the 2D map showing the evolution of the coordinate-dependent probability distribution $|\Psi(\phi, t)|^2$ as a function of time. For this particular case the initial wavepacket is $\Psi(\phi, t = 0) = \sum_M C_M \psi_M(\phi)$ with a Gaussian distribution $C_M = \exp[-M^2/\Delta M^2]$, $\Delta M = 6$.

This state corresponds to an initially oriented rotor. In practice, an oriented state of a heteronuclear molecule can be created by a strong "half-cycle" terahertz pulse [22], or a combination of a DC electric field and an aligning laser pulse [23].

At $t = 0$ the wavepacket is localized at $\phi = 0$ (Fig.2(b)). The initial localization is quickly lost: the wavepacket spreads along the rotational orbit $\phi = -\pi..\pi$. However, the quantized nature of the spectrum leads to periodic re-localization of the wavepacket – the so-called revivals [20]. At the revival time

$$T_{rev} = 2\pi/B \tag{3}$$

the wavepacket revives exactly in its original form. At $T_{rev}/2$ it revives as an exact replica placed at the opposite side of the trajectory, $\phi = \pi$. For any odd N, at any T_{rev}/N the revival pattern consists of N equally spaced replicas with well defined relative phases, such as those shown in Fig.2(c). For even $N = 2K$, at T_{rev}/N the revival pattern consists of $K = N/2$ equally spaced replicas. These moments and their multiples are called "fractional revivals" [20].

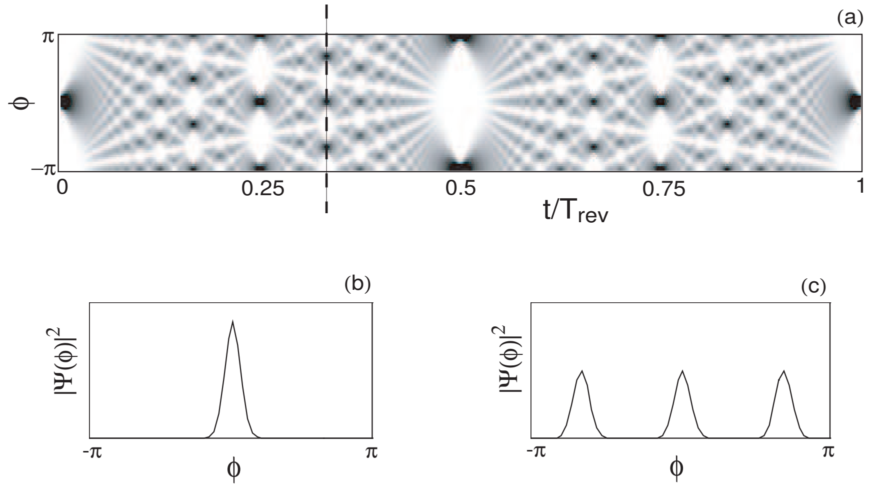

FIG. 2: (a): Density plot of evolution of the probability distribution for the angular wavepacket initially placed at $\phi = 0$ (b,c): Probability distribution at $t = 0$ and $t = T_{rev}/3$ (dashed line on the panel (a)), in arbitrary units.

The controllability criterium which we shall use below is based on the fact that in the wavepacket experiments one is usually interested in coarse-grained measures of *wavepacket localization*, rather than in a complete fine evolution of all quantum amplitudes. For example, for a rotational wave packet the commonly asked questions are whether the molecular wave packet is oriented in some direction or not, whether it is aligned parallel to some direction or not, how high is the degree of alignment or orientation, etc. In the same way, one can ask whether a vibrational molecular wave packet is in the Frank-Condon region or not, whether or not a Rydberg electron is near the core where it can be ionized, etc. One is also interested in the degree of wavepacket localization in a region of interest. The approach explored below controls such integral properties of the wavepacket localization on progressively finer scales.

Figs. 3(a,b) show evolution of the commonly used measures of rotational orientation and alignment, $\langle\Psi(t)|\cos\phi|\Psi(t)\rangle$ and $\langle\Psi(t)|\cos^2\phi|\Psi(t)\rangle$. They illustrate the fact that the characteristic features in the wavepacket localization are most distinct at the moments of fractional revivals, where the wavepacket is re-localized into several replicas.

Consider for definiteveness the case of odd N. Since the pattern on the quantum carpet at $t > T_{rev}/N$ is determined by the relative phases of the wavepacket replicas at the moment of fractional revival $t = T_{rev}/N$, the intuitive idea is to control the wavepacket evolution by inducing relative phase shifts between these replicas at $t = T_{rev}/N$, [25, 26]. Applying phase

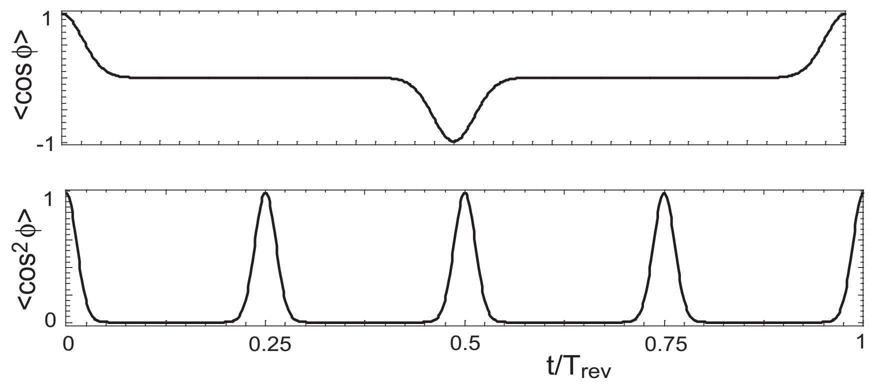

FIG. 3: Time evolution of the measures of orientation and alignment for the wavepacket shown on Fig.3.

shifts at fractional revivals creates superpositions of N equally spaced replicas of the original wavepacket, and thus controls the evolution with the accuracy of $1/N$-th of the orbit.

By *"coarse-grained controllability"*, for a given N, we shall mean that one can implement arbitrary unitary transform in the basis of N equally spaced replicas of the initial spatially localized wavepacket. Thus, arbitrary superposition of these replicas can be created. Spatial structure at the scale finer than $1/N$ is not resolved and is of no interest. The total number of levels involved in the dynamics is not specified – it is only relevant for structures with the scale finer than $1/N$. The coarse-grained basis will remain the same even if the dynamics involves increasing number of levels, but each basis wavepacket will change its shape at the sub-$1/N$ scale.

Phase shifts required in our control scheme can be implemented by coordinate-dependent interaction with a permanent or induced dipole moment triggered by a short pulse. Indeed, let $\hat{H}_0$ be the field-free Hamiltonian and $V(\phi,t) = V_0(t)v(\phi)$ the interaction with the external field, applied over a very short time T. If the field-free motion during T is negligible, $H_0 T \ll 1$, then the propagator is reduced to the coordinate-dependent phase shift:

$$\hat{U}(T) = e^{-i\int_0^T(\hat{H}_0+V(\phi,t))dt} \approx e^{-iv(\phi)\int_0^T V_0(t)dt} = e^{-iAv(\phi)} \tag{4}$$

Physically, each of the laser pulses must be shorter than the period of linear motion of the wavepacket. As shown by examples in Refs. [25, 26], this condition can be easily satisfied within the current femtosecond technology. Note that for induced dipole $V_0(t) \propto E^2(t)$ and thus the integral in Eq.(4) is always non-zero. In the case of a permanent dipole one needs the so-called "half-cycle pulses" [24].

For the interaction with a permanent dipole moment $v(\phi) \propto \cos\phi_{MR}$ and for the non-resonant AC Stark shifts $v(\phi) \propto \cos^2\phi_{MR}$, where ϕ_{MR} is the angle between the molecular (rotor) axis and the polarization of the radiation. Using two orthogonal polarizations along X and Y axis, one obtains $v(\phi) \propto \cos\phi$ and $v(\phi) \propto \sin\phi$ for the interaction with the permanent dipole moment and $v(\phi) \propto \cos^2\phi$ and $v(\phi) \propto \sin^2\phi$ for the interaction with the induced dipole moment. The relationship $2\cos^2\phi - 1 = \cos 2\phi$ shows that rescaling the rotational constant B and a simple variable substitution reduce the second case to the first one. Thus, without loss of generality, we can limit our discussion to the case of a permanent dipole moment. In the following, we will allow two mutually orthogonal polarizations, thus having $\sin\phi$ and $\cos\phi$ phase profiles at our disposal.

Intuitively, it is clear that the suggested control mechanism should work if the phase is (i) imprinted onto each replica of the original wavepacket *as a whole*, and (ii) each wavepacket replica can acquire arbitrary phase relative to others. Such an ideal situation would be approached if either the Stark shift had a stepwise rather than smooth $\sin\phi$ or $\cos\phi$ shape, or if the wavepackets in ϕ-representation were infinitely narrow. This ideal case was considered in [25, 26]. Here, we focus on the realistic case of a smooth phase profile and make no assumptions about how narrow the wavepacket replicas are.

Coarse-grained control up to $1/N$-th of the orbit implies the ability to generate all spatial modulations from $\sin\phi$ and $\cos\phi$ to $\sin N\phi$ and $\cos N\phi$ (or to $\sin^N\phi$ and $\cos^N\phi$). Intuitively, it is clear that having $\sin\phi$ and $\cos\phi$ phase profiles *in the exponent* and the ability to adjust the strength of the interaction A in Eq.(4) should enable us to generate all required spatial modulations. Indeed, $\exp(-iA\sin\phi) = \Sigma J_M(A)\exp(-iM\phi)$ contains all required harmonics with amplitudes $J_M(A)$ significantly different from zero for $M \lesssim A$ (J_M are the Bessel functions). The next two sections describe rigorous mathematical analysis that proves this intuitive statement. For the sake of simplicity we consider the case of odd N; the case of even N is slightly more cumbersome.

III. MATHEMATICAL FORMULATION OF THE PROBLEM

Suppose that the initial state in the energy basis is given by some vector $C(M)$. Then in the ϕ-representation the initial state of the system is

$$\Psi_0(\phi) = \frac{1}{\sqrt{2}} \sum_{M=-\infty}^{\infty} C(M) e^{iM\phi}. \tag{5}$$

At the fractional revival T_{rev}/N, N odd, $\Psi_0(\phi)$ breaks into N equally spaced replicas $\Psi_0(\phi - 2\pi l/N)$ with equal amplitudes $F_l^{(0)}$:

$$\Psi(\phi, T_{rev}/N) = \sum_{l=0}^{N-1} F_l^{(0)} * \Psi_0(\phi - \frac{2\pi l}{N}), \quad \text{where } |F_l^{(0)}|^2 = 1/N \tag{6}$$

Our goal is to be able to implement arbitrary transform acting on such superpositions, producing superpositions of the type

$$\Psi_{transformed}(\phi) = \sum_{l=0}^{N-1} F_l * \Psi_0(\phi - \frac{2\pi l}{N}), \quad \text{where } \sum_l |F_l|^2 = 1 \tag{7}$$

with arbitrary complex amplitudes F_l restricted only by the normalization condition. Then we will have achieved the desired coarse-grained controllability.

The transformed state in Eq.(7) is expressed in the energy basis as

$$C(M)_{transformed} = C(M) * D(M), \quad \text{where } D(M) = \sum_{l=0}^{N-1} F_l \, e^{2\pi i M l/N}. \tag{8}$$

Note that according to Eq.8 $D(M) = D(M+N)$. Such periodicity in the energy basis is the consequence of our coarse-grained approach. Being able to implement an arbitrary coarse-grained transform on $\Psi(\phi)$ is equivalent to being able to generate arbitrary, but N-periodic unitary transform acting on $D(M)$. Thus, in the energy basis, our goal is to be able to generate an infinite-dimensional block-diagonal matrix of the type

$$\begin{pmatrix} \ddots & & & & \\ & A_0 & & & \\ & & A_0 & & \\ & & & A_0 & \\ & & & & \ddots \end{pmatrix}, \tag{9}$$

where A_0 is an arbitrary unitary matrix of the size $N \times N$.

To implement the control, we use the free propagation Hamiltonian $H_0 = \mathrm{diag}(\ldots, E_{M-1}, E_M, E_{M+1}, \ldots)$, where $E_M = BM^2$, as well as H_1, H_2 that correspond to applying short pulses of vertical and horizontal polarization, imparting $\cos\phi$ and $\sin\phi$ phase profiles as explained in the previous section. In the energy basis, the Hamiltonians H_1 and H_2 are tridiagonal:

$$H_1 = \frac{1}{2}\begin{pmatrix} \cdot & \cdot & \cdot & & & \\ 1 & 0 & 1 & & & \\ & 1 & 0 & 1 & & \\ & & 1 & 0 & 1 & \\ & & & \cdot & \cdot & \cdot \end{pmatrix}, \quad H_2 = \frac{1}{2}\begin{pmatrix} \cdot & \cdot & \cdot & & & \\ -i & 0 & i & & & \\ & -i & 0 & i & & \\ & & -i & 0 & i & \\ & & & \cdot & \cdot & \cdot \end{pmatrix}. \quad (10)$$

We consider the evolution operator $\exp(i\hat{H}_0 t)$, but only for discrete set of times – the multiples of $\tau_0 = T_{rev}/N = \frac{2\pi}{BN}$, where N is a fixed odd positive integer. The evolution operator $\hat{g} = \exp(i\hat{H}_0\tau_0)$ is represented by a diagonal matrix $g = \mathrm{diag}(\ldots, \zeta^{(M-1)^2}, \zeta^{M^2}, \zeta^{(M+1)^2}, \ldots)$, where $\zeta = e^{\frac{2\pi i}{N}}$ is an N-th root of 1.

In the next section we show that the evolution operators for H_1 and H_2 together with g are sufficient to generate an even wider group of the infinite, unitary, periodic block matrices of the type

$$\begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & A_0 & A_1 & \cdot & \cdot \\ \cdot & A_{-1} & A_0 & A_1 & \cdot \\ \cdot & \cdot & A_{-1} & A_0 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix}. \quad (11)$$

We shall also discuss the condition of remaining within the sub-group represented by the block-diagonal matrices (9).

Mathematically, all possible $N \times N$ matrices in Eq.(9) belong to the SU_N group – the group of unitary matrices with the determinant equal to unity: $\overline{A}^T A = I$, $\det(A) = 1$. Here A^T is the transpose of A and $\overline{A}$ is its complex conjugate. In the infinite-dimensional Hilbert space, matrices Eq.(9) describe rotations in all directions within the limits imposed by the block-diagonal nature of these matrices and the SU_N-nature of the blocks.

In the following Section we show that, having matrices corresponding to the free evolution over the $1/N$ fractional revival and the phase kicks, we can make (infinitesimal) steps in any direction in the infinite-dimensional Hilbert space within the limits of the group of matrices given by Eq.(11). These matrices form an infinite-dimensional matrix representation of the so-called $SU_N[z, z^{-1}]$ loop group [27].

The $SU_N[z, z^{-1}]$ loop group is the set of all $N \times N$ matrices A whose entries are not numbers but complex polynomials in z, z^{-1}, with the conditions $\overline{A}^T A = I$ and $\det(A) = 1$. For the formal parameter z, there is a convention $\overline{z} = z^{-1}$: taking conjugate of a matrix whose elements are polynomials of z, we take complex conjugates of the numerical coefficients and replace z by z^{-1}. If z is moving along a unit circle in the complex plane, the convention $\overline{z} = z^{-1}$ is natural. For every fixed value of z, the matrix from $SU_N[z, z^{-1}]$ becomes a conventional matrix from SU_N. When we let z run over the unit circle, the corresponding matrix makes a loop in SU_N. This interpretation of loop groups is used in the string theory [28].

Alternatively, an element A of $SU_N[z, z^{-1}]$ can be viewed as a polynomial $A = \sum_k A_k z^k$ in powers of z and z^{-1}. In the infinite-dimensional matrix representation of $SU_N[z, z^{-1}]$ given by Eq.(11), the A_0 blocks go on the main diagonal, A_{-1} go just below it, A_1 just above it, etc.

IV. GEOMETRIC ANALYSIS

Mathematically, our goal is to show that our physical tools allow us to make infinitesimal steps in any direction staying within the limits of $SU_N[z, z^{-1}]$ – that is, to generate any element of the corresponding Lie algebra $su_N[z, z^{-1}]$. With the ability to move in arbitrary direction we should be able to approximate any element of the group. For finite-dimensional Lie groups the Lie correspondence theorem guarantees that the whole group of transformations can be generated if all of its Lie algebra is available. In the infinite-dimensional theory no analogue of such a theorem has been yet obtained. Nonetheless, we can expect that having the Lie algebra $su_N[z, z^{-1}]$ will allow us to approximate any element of the infinite-dimensional group $SU_N[z, z^{-1}]$.

The proof includes two theorems. Theorem 1 identifies a limited set of matrices which can be used to generate any element from $SU_N[z, z^{-1}]$. Theorem 2 shows how we can make (infinitesimal) steps towards any of the matrices from this set, identifying the required sequences of the free evolution and phase kicks. Thus, relying on the Theorem 1, the Theorem 2 proves that we can generate the Lie algebra $su_N[z, z^{-1}]$.

Theorem 1. The group $SU_N[z,z^{-1}]$ is generated by the following N subgroups, each isomorphic to SU_2:

$$\begin{pmatrix} a & b & & & & \\ c & d & & & & \\ & & 1 & & & \\ & & & \cdot & & \\ & & & & \cdot & \\ & & & & & 1 \end{pmatrix}, \begin{pmatrix} 1 & & & & & \\ & a & b & & & \\ & c & d & & & \\ & & & 1 & & \\ & & & & \cdot & \\ & & & & & 1 \end{pmatrix}, \dots \begin{pmatrix} 1 & & & & & \\ & \cdot & & & & \\ & & \cdot & & & \\ & & & 1 & & \\ & & & & a & b \\ & & & & c & d \end{pmatrix},$$

$$\begin{pmatrix} a & & & & & bz^{-1} \\ & 1 & & & & \\ & & \cdot & & & \\ & & & \cdot & & \\ & & & & 1 & \\ cz & & & & & d \end{pmatrix}, \tag{12}$$

with $\begin{pmatrix} a & b \\ c & d \end{pmatrix} \in SU_2$.

The proof of this Theorem is given in the Appendix.

Let us return to the Hamiltonians H_0, H_1, H_2. We see that the infinite matrix $g = \exp\left(iH_0 T_{rev}/N\right)$ is N-periodic, and can be identified with an element of $SU_N[z,z^{-1}]$. The matrices iH_1, iH_2 are also N-periodic and belong to the Lie algebra $su_N[z,z^{-1}]$.

Theorem 2. Let N be an odd integer. The operators $\{g^m(iH_1)g^{-m}, g^m(iH_2)g^{-m}\}$ where $m = 1, \dots N$ generate the Lie algebra $su_N[z,z^{-1}]$.

Proof. In Theorem 1 we showed that the Lie group $SU_N[z,z^{-1}]$ is generated by the set of matrices Eq.(12). This implies that the corresponding Lie algebra $su_N[z,z^{-1}]$ is generated by their $2N$ infinitesimal generators

$$\begin{pmatrix} 0 & i & & & & \\ i & 0 & & & & \\ & & 0 & & & \\ & & & \cdot & & \\ & & & & \cdot & \\ & & & & & 0 \end{pmatrix}, \begin{pmatrix} 0 & 1 & & & & \\ -1 & 0 & & & & \\ & & 0 & & & \\ & & & \cdot & & \\ & & & & \cdot & \\ & & & & & 0 \end{pmatrix}, \begin{pmatrix} 0 & & & & & \\ & 0 & i & & & \\ & i & 0 & & & \\ & & & 0 & & \\ & & & & \cdot & \\ & & & & & 0 \end{pmatrix},$$

$$\begin{pmatrix} 0 & & & & & \\ & 0 & 1 & & & \\ & -1 & 0 & & & \\ & & & \cdot & & \\ & & & & \cdot & \\ & & & & & 0 \end{pmatrix}, \ldots \begin{pmatrix} 0 & & & & & \\ & 0 & & & & \\ & & \cdot & & & \\ & & & \cdot & & \\ & & & & 0 & i \\ & & & & i & 0 \end{pmatrix}, \begin{pmatrix} 0 & & & & & \\ & 0 & & & & \\ & & \cdot & & & \\ & & & \cdot & & \\ & & & & 0 & 1 \\ & & & & -1 & 0 \end{pmatrix},$$

$$\begin{pmatrix} 0 & & & & & iz^{-1} \\ & 0 & & & & \\ & & \cdot & & & \\ & & & \cdot & & \\ & & & & 0 & \\ iz & & & & & 0 \end{pmatrix}, \begin{pmatrix} 0 & & & & & z^{-1} \\ & 0 & & & & \\ & & \cdot & & & \\ & & & \cdot & & \\ & & & & 0 & \\ -z & & & & & 0 \end{pmatrix}. \tag{13}$$

Below we show that the infinite matrices associated with these particular generators from $su_N[z, z^{-1}]$ can be written as the linear combinations

$$\sum_{m=1}^{N} \alpha_m g^m (iH_1) g^{-m} + \sum_{m=1}^{N} \beta_m g^m (iH_2) g^{-m}, \quad \text{with} \quad \alpha_m, \beta_m \in \mathbb{R}. \tag{14}$$

The matrices $g^m(iH_{1,2})g^{-m}$ are all tridiagonal, with zeroes on the main diagonal, and are determined by their upper-triangular parts, because of the condition $\overline{A}^T = -A$. The upper-triangular parts of $g^m(iH_1)g^{-m}$, $g^m(iH_2)g^{-m}$ are

$$\frac{i}{2} \sum_{j \in \mathbb{Z}} \zeta^{m(-2j+1)} E_{j,j+1} \quad \text{and} \quad -\frac{1}{2} \sum_{j \in \mathbb{Z}} \zeta^{m(-2j+1)} E_{j,j+1},$$

Here $E_{j,j+1}$ is a matrix that has the entry $\{j, j+1\}$ equal to 1, and all other entries are equal to 0, and $\zeta = \exp(2\pi i/N)$ is a complex N-th root of unity.

We use the identity that holds for odd N:

$$\sum_{m=1}^{N} \zeta^{m(2k-1)} \zeta^{m(-2j+1)} = \begin{cases} N, k = j \mod N \\ 0, \text{otherwise} \end{cases}. \tag{15}$$

(a sum of all the N different powers a complex root of 1, $\zeta^{(2k-1)}\zeta^{(-2j+1)}$, is equal to zero unless this root itself is equal to one).

Thus for $k = 1, \ldots, N$, the expressions

$$\frac{2}{N} \sum_{m=1}^{N} -\mathrm{Re}\zeta^{m(2k-1)} (g^m (iH_2) g^{-m}) + \mathrm{Im}\zeta^{m(2k-1)} (g^m (iH_1) g^{-m}) \tag{16}$$

will indeed give all the required generators. This completes the proof of the theorem.

In the language of laser pulses, Equations (14,16) imply that for every possible m we wait until the fractional revival g^{-m}, then apply the laser pulse of the horizontal or vertical polarization — H_1 or H_2 – and then apply g^m by waiting until the full revival. We can as well apply H_1 and H_2 simultaneously, so that Eq.(14) looks as

$$\sum_{m=1}^{N} g^m(i\alpha_m H_1 + i\beta_m H_2)g^{-m}, \qquad \alpha_m, \beta_m \in \mathbb{R}. \tag{17}$$

These correspond to applying linearly polarized pulses, with the angle of polarization defined by α_m/β_m. To generate each of the N matrices in Eq.(13), we can use N different pulses applied at N fractional revivals, and with the polarizations defined in Eq.(16). Since N is odd, we would use N different orientations of the field polarization in the plane. Even N would lead to only $N/2$ different polarizations and make the mathematical proof more complicated. In particular, phase kicks at multiples of $T_{rev}/2N$ would be needed. However, even before any proof, in practice for any $N = 2K$ one would be satisfied with controllability for $N = 2K - 1$ and $N = 2K + 1$. Of course, in practice one also does not have to use such complex pulse sequences; we only rely on them here for the sake of the mathematical proof.

V. CONCLUSIONS AND DISCUSSION

The main result of this paper is that wavepackets *are* coarse-grained controllable by free evolution and phase kicks given even by *smooth* coordinate-dependent interactions such as non-resonant Stark shifts. The two polarizations of the laser field, creating $H_1 \sim \cos\phi$ and $H_2 \sim \sin\phi$, suffice to approximate, for any odd N, any evolution matrix of the type (11) – and, as a subset, any evolution matrix of the type (9), which corresponds to controllability with the accuracy up to $1/N$th of the orbit.

This statement about coarse-grained controllability does not answer the question about the final shape of N basis wavepackets. Is it possible to avoid the (undesirable) change in the shape of the basis wavepackets and the uncontrollable spreading of the initial wapepacket distribution $C(M)$, while still being to create arbitrary superposition of the wavepacket replicas such as given by Eq.(7)?

An intuitive prescription has been described in Section II: one would like to use the wavepackets which are as narrow as possible and/or phase shifts with profiles as sharp as possible.

It turns out that there is also the possibility of a general solution of this problem. Within the group $SU_N[z, z^{-1}]$ of the evolution matrices (11) that we are able to generate, the blocks A_i, $i \neq 0$, are responsible for changing the shapes of the basis wavepackets by mixing different blocks in the input state vector, while A_0 provides the desired control without changing the shapes of the basis wavepackets. It is the last two operators in the set of the generators (13) that lead to the generation of non-diagonal blocks in the evolution matrix. If one uses all the possible control generators in Eq.(16,17) except for those with $k = N-1, N$, then only the finite group SU_N , represented by the block-diagonal evolution matrices (9) will be generated. There is also another potential possibility: if a control sequence has taken us to an undesired dimension, it may be possible to find a proper sequence of the type (14,16,17), which will bring us back to the block-diagonal evolution matrix of the type (9).

These geometric considerations do not give any useful practical prescription for the control sequence. Long sequences of the type (14,16,17), with "infinitesimal" laser pulses, are not feasible. The theory only proves the possibility of noiseless control. To find a practical solution, one could use a numerical or an experimental optimization algorithm [3].

The above analysis can be extended to wavepackets in weakly nonlinear 1D systems. Consider evolution of a wavepacket $\Psi(t) = \sum_n C_n(t)\Psi_n$ centered around n_0 in a system with quadratic spectrum, $E(n) = E(n_0) + \omega_0(n-n_0) + \Omega(n-n_0)^2$. In the semiclassical approximation this wavepacket can be viewed as a carrier Ψ_{n_0} modulated by the envelope $f(\phi,t) = \sum_n C_n(t)e^{i\phi(n-n_0)}$ [29], where the angle ϕ is the phase of the corresponding classical motion. Linear motion of the wavepacket is given by ω_0, while spreading and revivals of the envelope are defined by Ω: $T_{rev} = 2\pi/\Omega$ [20]. To describe the distribution on the corresponding classical orbit, one can track the shape of the envelope shifted by linear motion, $\tilde{f}(\tilde{\phi},t) = \sum_n C_n(0)\mathrm{exp}[-i\Omega_0 t(n-n_0)^2]\mathrm{exp}[i\tilde{\phi}(n-n_0)]$, $\tilde{\phi} = \phi - \omega_0 t$. Evolution of $\tilde{f}(\tilde{\phi})$ is identical to that of the wavefunction of a 2D rotor above.

If the spreading of the wavepacket is much slower then its linear motion, then one can utilize the existence of two vastly different time scales for similar to using two different polarizations in the above analysis. Specifically, the same coordinate-dependent Stark shift can be applied at those moments of time when the original wavepacket is at $\phi = 0$ and when it is at $\phi = \pi$. This technique was used in Ref.[25] to model quantum logic gates in a vibrational molecular wavepacket.

Finally, let us comment on the connection of the control regime studied here with the field of quantum chaos. A 2D rotor, kicked periodically with the same kind of the kick – H_1 or H_2 of the fixed amplitude – is the most fundamental model system studied in that field [30]. It is well known that if the kick period is not commensurate with the wavepacket revival time, then the quantum kicked rotor follows the behavior of its classical counterpart until saturation of the diffusion due to dynamic localization [30, 31]. However, if the kicks are applied at fractional revivals, then the behaviour of the quantum kicked rotor is drastically different. In particular, average energy of the system grows quadratically rather then linearly with time.

On the one hand, the main difference between the general analysis developed here and the case of resonantly kicked rotor is that here the kicks are in general not periodic and not identical - the strengths, polarizations, and time-delay between the kicks can change.

On the other hand, to the best of our knowledge the theory of resonantly kicked rotor [32] has only been developed for kicks applied at full revivals. The role of interferences at fractional revivals, the width of the resonances and their role – all very important issues for the control of quantum chaotic systems [33] – are not known. We hope can that the geometric analysis introduced here – i.e. the knowledge of what kind of pulse sequences are responsible for the quick climbing along the momentum ladder (Eq.(16)) – could be useful in addressing these problems.

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VI. APPENDIX

Let us outline the proof of Theorem 1. First of all, using standard algebraic manipulations, one can show that the group generated by these SU_2 subgroups also contains the subgroups

$$\begin{pmatrix} \cdot & & & & & \\ & 1 & & & & \\ & & a & & bz^{-k} & \\ & & & \cdot & & \\ & & cz^{k} & & d & \\ & & & & & 1 \\ & & & & & & \cdot \end{pmatrix}, \tag{18}$$

as well as the diagonal matrices $\mathrm{diag}(z^{s_1}, \ldots, z^{s_N})$ with $s_1 + \ldots s_N = 0$.

Indeed, if in the first $N-1$ matrices in (12) we set $a = d = 0$, $b = -c = 1$, then we will be able to create an arbitrary permutation of basis vectors. Using permutations and the first matrix in (12) with a, b, c, d not fixed, we can mix any two vectors - i.e., create any matrix of the form (18) with $k = 0$. Adding the last matrix from the set (12), we can generate any matrix of the form (18).

Now we can prove the theorem by induction on N. To make the inductive step, we need to show that multiplying a given matrix in $SU_N[z, z^{-1}]$ by matrices of the form (1), we can make the first column to be

$$(1, 0, \ldots, 0)^T. \tag{19}$$

Since the matrix is unitary, this will force the first row to be $(1, 0, \ldots, 0)$, and the problem is reduced to matrices of size $N-1$. Again we shall use induction, now on the width of the column.

Dealing with a given single column, we shall sequentially use matrices of the form (18) to simplify it to the form (19).

Let us, first, define *width* of a polynomial $f(z) = \sum_{j=s}^{n} a_j z^j$ as $w(f) = n - s + 1$ (here we assume $a_n \neq 0$, $a_s \neq 0$). The width $w(C)$ of a column $C = (f_1(z), \ldots, f_N(z))^T$ is defined as the maximal width of its entries $f_i(z)$.

If in the column we have two different lines with polynomials of the maximal width, then we shall be able to mix them together so that the width in at least one of them will be reduced. The claim below guarantees that there could not be a situation when there is only one line with polynomial of maximal width.

Claim. If the width of a column C of a matrix in $SU_N[z, z^{-1}]$ is greater than 1, then the column contains at least two entries of the maximal width.

First, note that for a polynomial $f(z)=\sum\limits_{j=s}^{n} a_j z^j$, the highest power of z in the expression

$$\overline{f}(z)f(z)=\left(\sum_{j=s}^{n}\overline{a}_j z^{-j}\right)\left(\sum_{j=s}^{n}a_j z^j\right)$$

is $n-s=w(f)-1$. Note that $\overline{C}^T C=1$, which holds since the matrix is unitary. Hence, if the width of C is greater than 1, the terms of the highest power of z, $w(C)-1$, in $\overline{C}^T C=\sum_{i=1}^{N}\overline{f}_i(z)f_i(z)$ must cancel out. Thus there should be more than one entry of the maximal width.

Now it is easy to see that having two entries in C of maximal width, we can apply an appropriate matrix of the form (1) to reduce the number of entries of maximal width. Continuing by induction, we complete the proof of the theorem.

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