Symplectic completion of symplectic jets

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In this paper, we outline a method for symplectic integration of three degree-of-freedom Hamiltonian systems. We start by representing the Hamiltonian system as a symplectic map. This map (in general) has an infinite Taylor series. In practice, we can compute only a finite number of terms in this series. This gives rise to a truncated map approximation of the original map. This truncated map is however not symplectic and can lead to wrong stability results when iterated. In this paper, following a generalization of the approach pioneered by Irwin (SSC Report No. 228, 1989), we factorize the map as a product of special maps called ''jolt maps'' in such a manner that symplecticity is maintained. © *1996 American Institute of Physics.* [S0022-2488(96)03509-8]

I. INTRODUCTION

Consider a complicated periodic Hamiltonian system that is non-integrable. Suppose we are interested in the long-term stability of particles being transported through this system. Since the system is assumed to be nonintegrable, it is very difficult to give stability criteria in an analytic form. A possible solution is to numerically follow the trajectories of particles through the system for a large number of periods (a process that goes by the name of tracking). One could then attempt to infer the stability of motion in the system by analyzing these tracking results.

The most straightforward method that can be used to perform this long term tracking is numerical integration. However, this method is too slow for analyzing the stability of very complicated systems. Therefore, we need a method that is both fast and accurate.

Several symplectic integration methods have been discussed in the literature. Ruth,[1] Feng,[2] Channel and Scovel,[3] Yoshida,[4] Berg *et al.*[5] and others have derived symplectic integrators using generating functions. These are typically implicit methods and using these methods requires one to use Newton's method with its attendent questions of convergence, etc. Another approach is through solvable maps.[6,7] But this method has not been explored in great detail. In this paper, following Irwin,[8] we explore a more direct method of symplectic integration.

The method that we will use is the iteration of symplectic maps[9] representing the Hamiltonian system. We start by defining certain mathematical objects. Let us denote the collection of six phase space variables q_i, p_i $(i=1,2,3)$ by the symbol z:

$$z=(q_1,p_1,q_2,p_2,q_3,p_3). \tag{1.1}$$

The Lie operator corresponding to a phase space function $f(z)$ is denoted by $:f(z):$. It is defined by its action on a phase-space function $g(z)$ as shown below

$$:f(z):g(z)=[f(z),g(z)]. \tag{1.2}$$

Here $[f(z),g(z)]$ denotes the usual Poisson bracket of the functions $f(z)$ and $g(z)$. Next, we define the exponential of a Lie operator. It is called a Lie transformation and is given as follows:

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$$e^{:f(z):}=\sum_{n=0}^{\infty}\frac{:f(z):^n}{n!}. \tag{1.3}$$

Powers of $:f(z):$ that appear in the above equation are defined recursively by the relation

$$:f(z):^n g(z)=:f(z):^{n-1}[f(z),g(z)], \tag{1.4}$$

with

$$:f(z):^0 g(z)=g(z). \tag{1.5}$$

For further details regarding Lie operators and Lie transformations, see Ref. 9.

The time evolution of the Hamiltonian system over one period can be represented by a symplectic map $\mathcal{M}$.[9] Symplectic maps are maps whose Jacobian matrices $M(z)$ satisfy the following symplectic condition:

$$\widetilde{M(z)}JM(z)=J, \tag{1.6}$$

where $\widetilde{M}$ is the transpose of M and J is an antisymmetric matrix defined as follows:

$$J=\begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & -1 & 0 \end{pmatrix}. \tag{1.7}$$

Matrices M satisfying Eq. (1.6) are called symplectic matrices and the corresponding maps $\mathcal{M}$ symplectic maps. It can be shown[9] that the set of all $\mathcal{M}$'s forms an infinite dimensional Lie group of symplectic maps. On the other hand, the set of all real 6×6 symplectic matrices forms the finite dimensional real symplectic group Sp(6,R).

Using the Dragt–Finn factorization theorem,[9,10] the symplectic map $\mathcal{M}$ can be factorized as shown below:

$$\mathcal{M}=\hat{M}e^{:f_3:}e^{:f_4:}\ldots e^{:f_n:}\ldots . \tag{1.8}$$

Here $\hat{M}$ gives the linear part of the map and hence has an equivalent representation in terms of the Jacobian matrix $M(0)$ of the map $\mathcal{M}$ at the origin:[9]

$$\hat{M}z_i=M_{ij}z_j=(Mz)_i. \tag{1.9}$$

Thus, $\hat{M}$ is said to be the Lie transformation corresponding to the 6×6 matrix M belonging to Sp(6,R). The infinite product of Lie transformations $\exp(:f_n:)$ $(n=3,4,\ldots)$ in Eq. (1.8) represents the nonlinear part of $\mathcal{M}$. Here $f_n(z)$ denotes a homogeneous polynomial (in z) of degree n uniquely determined by the factorization theorem.

The above map $\mathcal{M}$ is called the one-period map for the system. It gives the final state $z^{(1)}$ of a particle after one period as a function of its initial state $z^{(0)}$:

$$z^{(1)}=\mathcal{M}z^{(0)}. \tag{1.10}$$

To obtain the state of a particle after N periods, one has to merely iterate the above mapping N times, i.e.,

$$z^{(N)}=\mathcal{M}^N z^{(0)}. \tag{1.11}$$

It is obvious that one cannot use $\mathcal{M}$ in the form given in Eq. (1.8) for any practical computations. It involves an infinite number of Lie transformations. Therefore, we have to truncate $\mathcal{M}$ by stopping after a finite number of Lie transformations:

$$\mathcal{M}\approx \hat{M}e^{:f_3:}e^{:f_4:}\ldots e^{:f_P:}. \tag{1.12}$$

However, we are still not out of the woods. Each exponential $e^{:f_n:}$ in $\mathcal{M}$ contains an infinite number of terms in its Taylor series expansion. One possible solution is to truncate the Taylor series generated by the Lie transformations to order P. We denote this truncated map by $\mathcal{M}_P$. As a power series in the six phase space variables, it is given as follows:

$$\mathcal{M}_P z=M(1+:f_3:+\cdots)(1+:f_4:+\cdots)$$
$$\cdots(1+:f_p:+\cdots)z, \tag{1.13}$$

where we have to truncate the power series in such a way that the highest order term generated is z^{P-1}. If we did not impose this restriction, we would generate terms of order z^P and higher. Then, to be consistent, we would be forced to include in our map, $:f_n:$'s for n greater than P (since these also generate terms of order z^P and higher).

Equation (1.13) can be rewritten as follows:

$$\mathcal{M}_P z=h_1(z)+h_2(z)+\cdots+h_{P-1}(z), \tag{1.14}$$

where $h_n(z)$ denotes a polynomial of degree n in z. Since we have decided to consistently drop terms of order z^P and higher, we can define the following equivalence relation between maps of order P:

$$\mathcal{M}_P\sim\mathcal{M}'_P \quad \text{if } \mathcal{M}_P z-\mathcal{M}'_P z=h_P(z)+\text{higher order terms}. \tag{1.15}$$

This can be rephrased in terms of partial derivatives as follows. Maps $\mathcal{M}_P$ and $\mathcal{M}'_P$ are equivalent if all the partial derivatives of $\mathcal{M}_P z$ and $\mathcal{M}'_P z$ up to order $P-1$ are equal. An equivalence class with respect to this equivalence relation is called a jet of order P. Since the map $\mathcal{M}_P$ is obtained from a symplectic map $\mathcal{M}$, we call $\mathcal{M}_P$ (or more accurately, the equivalence class to which it belongs) a symplectic jet of order P. We stress that, despite its name, $\mathcal{M}_P$ is not symplectic.

We note that symplectic jets of order P have the following properties. A symplectic jet maps $\mathbb{R}^6$ into $\mathbb{R}^6$. It maps the origin of $\mathbb{R}^6$ into itself. It is invertible. And the composition of two symplectic jets $\mathcal{M}_P$ and $\mathcal{M}'_P$ is defined as follows:

$$\mathcal{M}_P\cdot\mathcal{M}'_P=(\mathcal{M}\cdot\mathcal{M}')_P. \tag{1.16}$$

This is again a symplectic jet of order P. And finally, there exists an identity given by the following equivalence class:

$$\mathcal{M}^0_P z=z+h_P(z)+\text{higher order terms}. \tag{1.17}$$

Therefore, the set of all symplectic jets of order P forms a group. It can be shown that it is actually a Lie group. This Lie group formed by the set of all symplectic jets of order P is called the symplectic jet group Spj(6;P).

However, the above solution of truncating the Taylor series has a severe shortcoming. As mentioned above, the mapping $\mathcal{M}_P$ generated by the truncated Taylor series is no longer symplectic. Therefore, repeated iterations of this mapping can lead to spurious growth (or damping) in the amplitude of motion of the particle being tracked. Obviously, this can lead to wrong conclusions regarding the stability of the system. Therefore it is important to preserve the symplectic nature of $\mathscr{M}_P$ when using it for long term tracking. For this purpose, we need to ensure that each factor in $\mathscr{M}_P$ takes the form $e^{:g:}$. On the other hand, for the numerical tracking scheme to be practical, we need to ensure that we evaluate only a finite number of terms. In this paper, we discuss how to reconcile these two apparently contradictory objectives.

The basic goal of this paper is to refactorize $\mathscr{M}_P$ [cf. Eq. (1.13)] as a product of symplectic maps that can be evaluated exactly. Since we do not truncate the Taylor series, we preserve the symplectic nature of the map even when we evaluate it. Another attractive feature of these special maps is that their inverses can also be evaluated exactly. The process of refactorizing a map into a product of symplectic maps characterized by these nice features is called ''symplectic completion''. Since the map that is being refactorized is $\mathscr{M}_P$, a symplectic jet, this refactorization procedure is called ''symplectic completion of symplectic jets''. And this will be the subject of this paper.

We start by defining jolt maps in Section II. In Section III, we formulate the problem of symplectic completion of $\mathscr{M}_P$ in terms of these jolt maps. Here, we follow the procedure first outlined by Irwin.[8] To get a better understanding of the problem, we first solve a model problem in Section IV. In Section V, we formulate a solution to the problem of symplectic completion of symplectic jets. In Section VI, we optimize the number of jolt maps required so that an efficient numerical algorithm is obtained.

II. JOLT MAPS

Consider the symplectic map given by $e^{:g(z):}$ where $g(z)$ is a function of the phase space variables z. It is called a jolt map if $:g(z):$ is a nilpotent operator of rank 2, i.e., if the following condition is satisfied:

$$:g(z):^2 z = 0. \tag{2.1}$$

The function $g(z)$ is then called a jolt function. We note that jolt maps have only two nonzero terms in their Taylor series expansions [cf. Eq. (1.3)]. The term jolt map was first introduced in Ref. 11.

Examples of jolt maps are given by the following theorem.

Theorem 1: *The following maps are jolt maps*

$$\text{(i)}\quad \hat{R}e^{:q_1^n:}\hat{R}^{-1} = e^{:\hat{R}q_1^n:}, \tag{2.2}$$

$$\text{(ii)}\quad \hat{R}e^{:f(q_1,q_2,q_3):}\hat{R}^{-1} = e^{:\hat{R}f(q_1,q_2,q_3):}. \tag{2.3}$$

Here $f(q_1,q_2,q_3)$ *is an nth degree polynomial in variables* q_1, q_2, *and* q_3. *Finally,* $\hat{R}$ *is the Lie transformation corresponding to a* 6×6 *matrix R belonging to any subgroup of* Sp(6,R) *[including* Sp(6,R) *itself]. It is given by the following relation [cf. Eq. (1.9)]:*

$$\hat{R}z_i = R_{ij}z_j = (Rz)_i . \tag{2.4}$$

See Appendix A for a proof of this theorem. In this theorem, note that the second statement contains the first statement as a special case. However, a separate (and simpler) proof is given even for the first statement since we will be using this later in the paper.

III. FORMULATION OF THE PROBLEM OF JOLT FACTORIZATION

Our goal is to refactorize $\mathscr{M}_P$ [cf. Eq. (1.13)] in terms of a finite number of jolt maps. The first step towards achieving this goal is to formulate the problem in an appropriate form. The best way to mathematically formulate the problem appears to be as follows[8]:

Problem 1: *Given the map $\mathscr{M}_P$, find another map $\mathscr{J}$ specified by the following product of K jolt maps*:

$$\mathscr{J}=\hat{M}e^{:g_3^{(1)}+g_4^{(1)}+\cdots+g_P^{(1)}:}e^{:g_3^{(2)}+g_4^{(2)}+\cdots+g_P^{(2)}:}\dots e^{:g_3^{(K)}+g_4^{(K)}+\cdots+g_P^{(K)}:} \tag{3.1}$$

such that this map agrees with $\mathscr{M}_P$ to order P, i.e.,

$$\mathscr{J}\cong\mathscr{M}_P \quad \text{to order } P. \tag{3.2}$$

Here $g_n^{(i)}$'s are (homogeneous) jolt polynomials of degree n given by the following relation:

$$g_n^{(i)}=\beta_n^{(i)}\hat{R}_i q_1^n, \quad i=1,2,\dots,K, \tag{3.3}$$

where $\beta_n^{(i)}$ is a real coefficient. The matrices R_i belong to a subgroup of Sp(6,R) *[including* Sp(6,R) *itself] and $\hat{R}_i$ denotes the Lie transformation corresponding to these matrices [cf. Eq. (2.4)].*

Before proceeding further, we note that Eq. (3.1) can be rewritten in the following form:

$$\mathscr{J}=\hat{M}e^{:g^{(1)}:}e^{:g^{(2)}:}\dots e^{:g^{(K)}:}, \tag{3.4}$$

where

$$g^{(i)}=g_3^{(i)}+g_4^{(i)}+\cdots g_P^{(i)} \quad i=1,2,\dots,K. \tag{3.5}$$

From Eq. (3.3) and Theorem 1 [cf. Eq. (2.2)] it is seen that $g^{(i)}$'s are jolt polynomials (a sum of jolt polynomials is easily shown to be another jolt polynomial). Consequently, $\exp(:g^{(i)}:)$'s are jolt maps.

In order to solve the above problem, we need to determine the various unknown quantities appearing in the above equations—the number of jolt maps K, the matrices R_i, and the coefficients $\beta_n^{(i)}$. It turns out that K and R_i can be determined independent of the details of the map $\mathscr{M}_P$. They depend only on the order P of the map. This will be explicitly demonstrated shortly. For the moment, we will assume that K and R_i have already been fixed. This reduces our task to merely finding the coefficients $\beta_n^{(i)}$'s such that Eq. (3.2) is satisfied. We now proceed to solve for these coefficients order by order.

Since the linear part of a symplectic map can be evaluated exactly, there is no need to refactorize it in terms of jolt maps. Hence, we have already chosen the linear parts of the maps $\mathscr{M}_P$ and $\mathscr{J}$ to be the same. Therefore, we need to refactorize only the nonlinear part of $\mathscr{M}_P$. We start by comparing terms of order 3 in $\mathscr{M}_P$ and $\mathscr{J}$ respectively. The third-order term in $\mathscr{M}_P$ is given by f_3. To obtain the third-order term in $\mathscr{J}$, we need to cast it in the standard Dragt–Finn form. This is accomplished by using the Baker–Campbell–Hausdorff (BCH) formula[10] given below:

$$\exp(t:f:)\exp(s:g:)=\exp(t:f:+s:g:+ts:[f,g]:/2+\cdots). \tag{3.6}$$

We get the following result to third order:

$$\mathscr{J}\cong\hat{M}e^{:h_3:}, \tag{3.7}$$

where

$$h_3 = \sum_{i=1}^{K} g_3^{(i)}. \tag{3.8}$$

Therefore, $\mathscr{J}$ and $\mathscr{M}_P$ will be equal to order 3 if the following equality is satisfied [cf. Eq. (3.3)]:

$$\sum_{i=1}^{K} \beta_3^{(i)} \hat{R}_i q_1^3 = f_3. \tag{3.9}$$

In other words, we have to determine $\beta_3^{(i)}$'s such that the above equation is satisfied.

Next, we compare terms of order 4 in $\mathscr{M}_P$ and $\mathscr{J}$. The fourth-order term in $\mathscr{M}_P$ is given by f_4. Using the BCH formula, the Dragt–Finn factorization of $\mathscr{J}$ correct to fourth order is given by the following result:

$$\mathscr{J} \cong \hat{M} e^{:h_3:} e^{:h_4:}, \tag{3.10}$$

where

$$h_4 = \sum_{i=1}^{K} g_4^{(i)} + \frac{1}{2} \sum_{j<k} [g_3^{(j)}, g_3^{(k)}]. \tag{3.11}$$

The second term on the right hand side of the above equation is a fourth-order term produced by the concatenation of third-order terms in Eq. (3.1). Equating the fourth-order terms of $\mathscr{M}_P$ and $\mathscr{J}$ we get the relation [cf. Eq. (3.3)]

$$\sum_{i=1}^{K} \beta_4^{(i)} \hat{R}_i q_1^4 = f_4 - \frac{1}{2} \sum_{j<k} \beta_3^{(j)} \beta_3^{(k)} [\hat{R}_j q_1^3, \hat{R}_k q_1^3] \equiv f_4'. \tag{3.12}$$

Here f_4' includes the fourth-order terms produced by concatenation of lower order terms. By choosing $\beta_4^{(i)}$'s such that the above equation is satisfied, we ensure that $\mathscr{J}$ and $\mathscr{M}_P$ agree to fourth order.

This process can be continued in a similar fashion to deal with the higher order terms. At the nth order, we have to choose $\beta_n^{(i)}$'s such that the following equality is satisfied:

$$\sum_{i=1}^{K} \beta_n^{(i)} \hat{R}_i q_1^n = f_n'. \tag{3.13}$$

Here f_n' includes the unwanted nth-order terms produced by $g_l^{(i)}$ $(l<n)$.

We are now in a position to determine the number of jolt maps K and the matrices R_i. We will show that they are independent of the map $\mathscr{M}_P$. We note that f_n' involves $N(n)$ independent coefficients where $N(n)$ is given by the relation[8]

$$N(n) = \binom{n+5}{n}. \tag{3.14}$$

Thus, we need at least $N(n)$ $\beta_n^{(i)}$'s to solve the above equation. Since $N(n)$ is a monotonically increasing function of n, the maximum number of $\beta_n^{(i)}$'s are required when n is equal to P (the maximum order). Thus we need $N(P)$ $\beta_n^{(i)}$'s to solve Eq. (3.13) for all n. This fixes K to be equal to $N(P)$. Moreover, $\hat{R}_i q_1^n$ $(i=1,\ldots,K)$ should be linearly independent quantities. This imposes restrictions on the matrices R_i that we can choose. Both these conditions are independent of f_n', i.e., they are independent of the map $\mathscr{M}_P$. They depend only on the maximum order P. Therefore both K and R_i's can be fixed in advance independent of the map to be represented.

Once K and the R_i's are fixed, we start by first solving Eq. (3.9) for $\beta_3^{(i)}$'s. We then proceed order by order until we reach the Pth-order equation. At the nth order, we have to solve Eq. (3.13). The right hand side involves $N(n)$ independent coefficients. Since $N(n)$ is less than K $(=N(P))$ for n less than P, we have more $\beta_n^{(i)}$'s than necessary to solve this equation, i.e., the $\beta_n^{(i)}$'s are underdetermined. The naive solution would be to set these extra $\beta_n^{(i)}$'s to zero

$$\beta_n^{(i)}=0 \quad \text{for } i>N(n). \tag{3.15}$$

But there is a better solution. We fix these extra $\beta_n^{(i)}$'s by requiring that $\Sigma_{i=1}^{K}(\beta_n^{(i)})^2$ be a minimum. The reason for this is simple. We have seen that the nth-order jolt polynomials produce higher order terms [for example, see Eq. (3.11)] upon concatenation. These higher order terms depend on the coefficients $\beta_n^{(i)}$ [for example, see Eq. (3.12)]. Therefore, by minimizing the sum of the squares of these coefficients, we reduce the magnitude of the unwanted higher order terms produced by concatenation of lower order terms.

Putting everything together, the problem of obtaining a jolt map factorization can be reduced to the following general problem:

Problem 2: *Given a nth degree homogeneous polynomial f_n and K matrices R_i, find the coefficients $\beta_n^{(i)}$'s such that the following conditions are satisfied:*

$$\text{(i)} \quad \sum_{i=1}^{K} \beta_n^{(i)}\hat{R}_i q_1^n = f_n \tag{3.16}$$

and

$$\text{(ii)} \quad \sum_{i=1}^{K} [\beta_n^{(i)}]^2 \text{ is a minimum.} \tag{3.17}$$

IV. A MODEL PROBLEM AND ITS SOLUTION

Before attempting to solve the general problem outlined above, we will first solve a model problem in this section. This model problem is deliberately designed to be quite similar to the problem of jolt factorization [cf. Eqs. (3.16) and (3.17)]. Therefore, solving this problem will enable us to get a feel for the issues involved in the solution of the jolt factorization problem.

Consider an arbitrary vector v in the two dimensional $x-y$ plane. It can be expressed as follows:

$$v=v_x e_x+v_y e_y, \tag{4.1}$$

where e_x and e_y are the usual unit vectors along the x and y axes, respectively, and v_x and v_y are the corresponding vector components. Next, we construct a new set of N basis vectors e_i (where N is an integer greater than 2) in the $x-y$ plane using the following procedure:

$$e_i=R(\theta_i)e_x, \quad i=1,2,\ldots,N, \tag{4.2}$$

where

$$R(\theta_i)e_x=\cos(\theta_i)e_x+\sin(\theta_i)e_y \tag{4.3}$$

and

$$\theta_i=(k-1)\,\frac{2\pi}{N}. \tag{4.4}$$

We are now in a position to state the problem—express v in the new basis given by the N e_i's. Of course, only two basis vectors are actually needed to express the vector v. Since we have extra basis vectors, we need to impose a constraint. Taking this into account, the problem can be formulated as follows.

Problem 3: *Given the vector v [cf. Eq. (4.1)], find coefficients β_i such that the following conditions are satisfied*:

$$\text{(i)} \quad v=\sum_{i=1}^{N} \beta_i e_i=\sum_{i=1}^{N} \beta_i R(\theta_i) e_x \tag{4.5}$$

and

$$\text{(ii)} \quad \sum_{i=1}^{N} \beta_i^2 \text{ is a minimum.} \tag{4.6}$$

The reader will immediately notice the striking similarity between this problem and the problem of jolt factorization [cf. Eqs. (3.16) and (3.17)].

Instead of solving this particular problem, we will solve the more general problem obtained by going to the continuum limit. Its solution will then contain the solution to the original (discrete) problem as a special case. The generalized problem is given as follows.

Generalized Problem 1: *Given the vector v [cf. Eq. (4.1)], find the function $g(\theta)$ such that the following conditions are satisfied:*

$$\text{(i)} \quad v=\frac{1}{2\pi}\int_0^{2\pi} d\theta\, g(\theta) R(\theta) e_x \tag{4.7}$$

and

$$\text{(ii)} \quad \frac{1}{2\pi}\int_0^{2\pi} d\theta\, g^2(\theta) \text{ is a minimum,} \tag{4.8}$$

where

$$R(\theta)e_x=\cos(\theta)e_x+\sin(\theta)e_y. \tag{4.9}$$

We solve this generalized problem as follows. We first find functions $g_x(\theta)$ and $g_y(\theta)$ satisfying the following relations:

$$\frac{1}{2\pi}\int_0^{2\pi} d\theta\, g_x(\theta) R(\theta) e_x=e_x, \tag{4.10}$$

$$\frac{1}{2\pi}\int_0^{2\pi} d\theta\, g_y(\theta) R(\theta) e_x=e_y. \tag{4.11}$$

In other words, the functions $g_x(\theta)$ and $g_y(\theta)$ project out the unit vectors e_x and e_y, respectively. Substituting Eq. (4.9) in the above expressions, we obtain the relations

$$\frac{1}{2\pi}\int_0^{2\pi} d\theta\, g_x(\theta)[\cos(\theta)e_x+\sin(\theta)e_y]=e_x, \tag{4.12}$$

$$\frac{1}{2\pi}\int_0^{2\pi} d\theta\, g_y(\theta)[\cos(\theta)e_x+\sin(\theta)e_y]=e_y. \tag{4.13}$$

The cosine and sine functions satisfy the following orthonormality conditions:

$$\frac{1}{2\pi}\int_0^{2\pi} d\theta\, \cos(m\theta)\cos(m'\theta)=\frac{1}{2}\,\delta_{mm'}+\frac{1}{2}\,\delta_{m0}\delta_{m'0}, \tag{4.14}$$

$$\frac{1}{2\pi}\int_0^{2\pi} d\theta\, \sin(m\theta)\sin(m'\theta)=\frac{1}{2}\,\delta_{mm'}-\frac{1}{2}\,\delta_{m0}\delta_{m'0}, \tag{4.15}$$

$$\frac{1}{2\pi}\int_0^{2\pi} d\theta\, \cos(m\theta)\sin(m'\theta)=0, \tag{4.16}$$

where m and m' are arbitrary integers. Using these orthonormality relations, we get the following solution for $g_x(\theta)$ and $g_y(\theta)$:

$$g_x(\theta)=2\cos(\theta); \quad g_y(\theta)=2\sin(\theta). \tag{4.17}$$

Consider the following function

$$g(\theta)=v_x g_x(\theta)+v_y g_y(\theta). \tag{4.18}$$

Substituting this function into the right hand side of Eq. (4.7), we get the following result:

$$\frac{1}{2\pi}\int_0^{2\pi} d\theta[v_x g_x(\theta)+v_y g_y(\theta)]R(\theta)e_x. \tag{4.19}$$

Using Eqs. (4.10) and (4.11), we obtain the relation [cf. Eq. (4.1)]

$$\frac{1}{2\pi}\int_0^{2\pi} d\theta\, g(\theta)R(\theta)e_x=v_x e_x+v_y e_y=v. \tag{4.20}$$

This proves that the function $g(\theta)$ given in Eq. (4.18) is a solution satisfying Eq. (4.7).

Next, we have to show that it also satisfies Eq. (4.8). Using the standard Fourier series expansion, the most general function satisfying Eq. (4.7) is found to be

$$g(\theta)=2v_x\cos(\theta)+2v_y\sin(\theta)+b_0+\sum_{n=2}^{\infty} b_n\cos(n\theta)+\sum_{n=2}^{\infty} a_n\sin(n\theta). \tag{4.21}$$

Using the orthonormality relations [cf. Eqs. (4.14), (4.15), and (4.16)], it is easily verified that this is indeed a solution to Eq. (4.7). Substituting this result into Eq. (4.8), we get the relation

$$\frac{1}{2\pi}\int_0^{2\pi} d\theta\, g^2(\theta)=2(v_x^2+v_y^2)+b_0^2+\sum_{n=2}^{\infty}(a_n^2+b_n^2)/2. \tag{4.22}$$

This is a minimum only if the following condition is satisfied:

$$b_0=0; \quad a_n=b_n=0 \quad n>1. \tag{4.23}$$

Imposing these conditions on the general solution [cf. Eq. (4.21)], we get back the particular solution given in Eq. (4.18). Thus, the function $g(\theta)$ displayed below is indeed the solution to the generalized problem stated in Eqs. (4.7) and (4.8):

$$g(\theta)=2v_x \cos(\theta)+2v_y \sin(\theta). \tag{4.24}$$

This solution satisfies the following relation [cf. Eqs. (4.22) and (4.23)]

$$\frac{1}{2\pi}\int_0^{2\pi} d\theta\, g^2(\theta)=2(v_x^2+v_y^2). \tag{4.25}$$

The discrete version of the generalized problem is given as follows: Given the vector v [cf. Eq. (4.1)], find values $g(\theta_i)$ $(i=1,2,\ldots,N)$ such that the following conditions are satisfied:

$$\text{(i)}\quad v=\frac{1}{N}\sum_{i=1}^{N} g(\theta_i)R(\theta_i)e_x \tag{4.26}$$

and

$$\text{(ii)}\quad \frac{1}{N}\sum_{i=1}^{N} [g(\theta_i)]^2 \text{ is a minimum.} \tag{4.27}$$

Comparing this with our original problem [cf. Eqs. (4.5) and (4.6)], we make the following identification:

$$\beta_i=g(\theta_i)/N. \tag{4.28}$$

If we choose the angles θ_i to be equally spaced over the interval $[0,2\pi]$ [as we did in the original problem, cf. Eq. (4.4)], $\cos(\theta_i)$ and $\sin(\theta_i)$ still form an othogonal set. Therefore, the solution $g(\theta)$ [cf. Eq. (4.24)] to the continuum problem is the solution even for the discrete version. The only difference is that $g(\theta)$ is now evaluated only at the discrete set of angles θ_i. Therefore, the coefficients β_i satisfying Eqs. (4.5) and (4.6) are given as follows [cf. Eqs. (4.24) and (4.28)]:

$$\beta_i=[2v_x \cos(\theta_i)+2v_y \sin(\theta_i)]/N. \tag{4.29}$$

The discrete version of Eq. (4.25) is found to be

$$\frac{1}{N}\sum_{i=1}^{N} [g(\theta_i)]^2=2(v_x^2+v_y^2). \tag{4.30}$$

Substituting Eq. (4.28) into this expression, we get the relation

$$\sum_{i=1}^{N} \beta_i^2=\frac{2}{N}(v_x^2+v_y^2). \tag{4.31}$$

We notice that the sum of the squares of the coefficients decreases as the number N of basis vectors increases. We also note that the basis vectors e_i [cf. Eq. (4.2)] form a discrete subgroup of the rotation group if the angles θ_i are equally spaced over the interval $[0,2\pi]$.

V. SOLUTION TO THE PROBLEM OF JOLT FACTORIZATION

In this section, we return to the problem of jolt factorization [cf. Eqs. (3.16) and (3.17)]. In Section II, we had concluded that the problem of obtaining a jolt factorization is equivalent to the determination of the coefficients $\beta_n^{(i)}$ subject to the conditions given in Eqs. (3.16) and (3.17). Hence, we will achieve our goal if we determine these $\beta_n^{(i)}$'s. However, in the previous section, we had discovered that the solution to such problems is facilitated by going over to the continuum limit. Therefore, we do the same for the problem of jolt factorization and obtain the following generalized problem.

Generalized Problem 2: *Given an nth degree homogeneous polynomial f_n and a subgroup G of* Sp(6,R) *on which invariant integration is well defined, find the function $g(u)$ such that the following conditions are satisfied:*

$$\text{(i)} \quad f_n = \int_G du\; g(u)\hat{R}(u) q_1^n \tag{5.1}$$

and

$$\text{(ii)} \quad \int_G du\; g^2(u) \quad \text{is a minimum.} \tag{5.2}$$

Here u denotes a general element of the group G and $\hat{R}(u)$ denotes the Lie transformation corresponding to u. All integrations are invariant integrations performed over the group G.

First we need to choose the group G. We cannot take G to be Sp(6,R) since Sp(6,R) is a noncompact group and therefore its invariant integrals cannot be normalized. We therefore integrate over a compact subgroup of Sp(6,R). The largest compact subgroup of Sp(6,R) is the unitary group U(3). However, we prefer to use SU(3) since it is more convenient for our purposes. If needed, it is possible to generalize the invariant integrals over SU(3) to those over U(3).

Having chosen G to be SU(3), we are now in a position to solve the problem. First, we notice the strong similarity between the present problem and the model problem that was solved in the previous section. Therefore, we will closely follow the procedure used to solve the model problem.

We need to determine the function $g(u)$. For this, we expand all quantities in terms of certain basis vectors. Since we are working with SU(3), it is natural that we use SU(3) basis vectors. Appendix B defines these basis vectors in terms of phase space variables (see Ref. 7 for additional details). Further, one can show[7] that any homogeneous polynomial f_n in the phase space variables can be decomposed in terms of these vectors.

We will denote by $|j;m\rangle$ the basis vectors uniquely labeled according to their transformation properties under SU(3). Here, j denotes the collection of indices j_1 and j_2 labeling the representation and m denotes the collection of indices I, I_3, and Y labeling vectors within the representation. (These basis vectors are analogous to the basis vectors e_x and e_y of the model problem.)

We expand the given homogeneous polynomial f_n in this basis as follows

$$f_n = \sum_{j,m} \phi_m^j |j;m\rangle \quad j \leq n. \tag{5.3}$$

A word on the notation used here. Since j stands for a collection of indices j_1 and j_2, $j \leq n$ actually means that $j_1 + j_2 \leq n$. Here, the ϕ_m^j's are coefficients multiplying the basis vectors. [This expansion is analogous to the one given in Eq. (4.1) for v in the model problem.] Thus, the left hand side of Eq. (5.1) has been expanded in terms of $|j;m\rangle$. However the right hand side is in terms of an integral over SU(3). Therefore, we will rewrite $|j;m\rangle$ in terms of an integral over SU(3) such that a direct comparison of the two sides is possible.

We proceed as follows. Suppose we can find a function $g_m^j(u)$ satisfying the following relation:

$$\int_{\mathrm{SU}(3)} du\; g_m^j(u)\hat{R}(u)q_1^n = |j;m\rangle, \quad j \leqslant n. \tag{5.4}$$

In other words, the function $g_m^j(u)$ projects out the basis vector $|j;m\rangle$. (This function is analogous to the functions g_x and g_y in the model problem.) Substituting this equation and Eq. (5.3) in Eq. (5.1) we get

$$\sum_{j,m} \phi_m^j \int_{\mathrm{SU}(3)} du\; g_m^j(u)\hat{R}(u)q_1^n = \int_{\mathrm{SU}(3)} du\; g(u)\hat{R}(u)q_1^n, \quad j \leqslant n. \tag{5.5}$$

Comparing both sides, we see that

$$g(u) = \sum_{j,m} \phi_m^j g_m^j(u), \quad j \leqslant n. \tag{5.6}$$

All that remains to be done is to determine $g_m^j(u)$ satisfying Eq. (5.4). To do this, we rewrite $\hat{R}(u)q_1^n$ in terms of SU(3) basis vectors. As a first step, we expand q_1^n in this basis (see Appendix B for a proof of this result):

$$q_1^n = \sum_{j \leqslant n} \xi^j |j;m_j\rangle. \tag{5.7}$$

We note two important features of this expansion (see Appendix B for a proof). First, the coefficients ξ^j are all nonzero:

$$\xi^j \neq 0, \quad j \leqslant n. \tag{5.8}$$

Second, each representation occurs *only* once. This is indicated by the fact that there is no summation over the indices m that label vectors within a representation. In summary, each representation (labeled by $j \leqslant n$) occurs once and only once in the expansion of q_1^n. This result will play a crucial role in the discussion that follows.

To get $\hat{R}(u)q_1^n$ we act on both sides of Eq. (5.7) with $\hat{R}(u)$, obtaining the following result:

$$\hat{R}(u)q_1^n = \sum_{j \leqslant n} \xi^j \hat{R}(u)|j;m_j\rangle. \tag{5.9}$$

Since the basis vectors $|j;m\rangle$ form a complete set for each j, they satisfy the relation

$$\sum_m |j;m\rangle\langle j;m| = 1 \quad \forall j. \tag{5.10}$$

Inserting this result into the right hand side of Eq. (5.9), we get the following relation:

$$\hat{R}(u)q_1^n = \sum_{j,m} \xi^j |j;m\rangle\langle j;m|\hat{R}(u)|j;m_j\rangle, \quad j \leqslant n. \tag{5.11}$$

However, we have the following standard result from representation theory of SU(3):

$$\langle j,m|\hat{R}(u)|j;m_j\rangle = \mathscr{D}^{\,j}_{mm_j}(u). \tag{5.12}$$

Substituting this into Eq. (5.11), we obtain the result

$$\hat{R}(u)q_1^n=\sum_{j,m}\xi^j\mathscr{D}^j_{mm_j}(u)|j;m\rangle,\quad j\leqslant n. \tag{5.13}$$

Inserting Eq. (5.13) into Eq. (5.4), we get the result

$$\int_{\mathrm{SU}(3)}du\ g_m^j(u)\sum_{j',m'}\xi^{j'}\mathscr{D}^{j'}_{m'm_{j'}}(u)|j',m'\rangle=|j;m\rangle,\quad j\leqslant n. \tag{5.14}$$

The functions $\mathscr{D}^j(u)$ satisfy the following orthogonality relations

$$\int_{\mathrm{SU}(3)}du\overline{\mathscr{D}}^j_{ab}(u)\mathscr{D}^{j'}_{a'b'}(u)=\frac{1}{d}\ \delta_{jj'}\delta_{aa'}\delta_{bb'}. \tag{5.15}$$

Here $\overline{\mathscr{D}}^j$ is the complex conjugate of the representation $\mathscr{D}^j$ and $d=(j_1+1)(j_2+1)\times((j_1+j_2)/2+1)$ is the dimension of the SU(3) representation labeled by j. Using these orthogonality relations, it is easily verified that the expression given below for $g_m^j(u)$ satisfies Eq. (5.14)

$$g_m^j(u)=\frac{d}{\xi^j}\ \overline{\mathscr{D}}^j_{mm_j}(u),\quad j\leqslant n. \tag{5.16}$$

We note that this expression is well defined since ξ^j is nonzero for $j\leqslant n$ [cf. Eq. (5.8)].

Having determined $g_m^j(u)$, we immediately obtain the required solution $g(u)$ [cf. Eq. (5.6)]:

$$g(u)=\sum_{j,m}\ \frac{d\phi_m^j}{\xi^j}\ \overline{\mathscr{D}}^j_{mm_j}(u),\quad j\leqslant n. \tag{5.17}$$

This is a solution satisfying Eq. (5.1). We need to verify that it also satisfies Eq. (5.2).

Again, we proceed as we did in the model problem. The most general solution $g(u)$ satisfying Eq. (5.1) is of the following form:

$$g(u)=\sum_{j,m}\ \frac{d\phi_m^j}{\xi^j}\ \overline{\mathscr{D}}^j_{mm_j}(u)+\sum_{j',a,b}c_{ab}^{j'}\overline{\mathscr{D}}^{j'}_{ab}(u). \tag{5.18}$$

Here the indices j', a, and b are required to satisfy the condition

$$\int_{\mathrm{SU}(3)}du\overline{\mathscr{D}}^{j'}_{ab}(u)\hat{R}(u)q_1^n=0. \tag{5.19}$$

This condition ensures that the extra terms added to obtain the general solution do not contribute to the integral in Eq. (5.1). However, these extra terms do contribute to the integral in Eq. (5.2). This is easily seen by substituting the general solution given in Eq. (5.18) into Eq. (5.2). We obtain the relation

$$\int_{\mathrm{SU}(3)}du\ g^2(u)=\sum_{j,m}\ d\left|\frac{\phi_m^j}{\xi^j}\right|^2+\sum_{j',a,b}\ |c_{ab}^{j'}|^2. \tag{5.20}$$

The above expression is minimized only if the following conditions are satisfied:

$$c_{ab}^{j'}=0\quad\forall j',a,b. \tag{5.21}$$

Imposing these conditions on the general solution [cf. Eq. (5.18)], we get back the particular solution given in Eq. (5.17). In summary, the function $g(u)$ given in Eq. (5.17) is the solution satisfying both Eqs. (5.1) and (5.2).

Having solved the problem in the continuum limit, we now return to the discrete version. Following the analogy with the model problem, we replace the integral over SU(3) by a sum over a discrete subgroup Γ of SU(3).[7] Since the elements of the discrete subgroups satisfy the same group properties as elements of the original group, the solution for the continuum problem would still be a solution to the discrete problem. There are several discrete subgroups of SU(3) that could be used. They are listed in detail in Appendix C. One should choose a subgroup of SU(3) whose order is greater than or equal to K. The above procedure leads us to the following result:

$$f_n=\frac{1}{K}\sum_{i=1}^{K} g(u_i)\hat{R}(u_i)q_1^n, \quad u_i\in\Gamma, \tag{5.22}$$

where $g(u)$ is given by Eq. (5.17). Comparing this with Eq. (3.16), we get the following solution for the coefficients $\beta_n^{(i)}$:

$$\beta_n^{(i)}=g(u_i)/K. \tag{5.23}$$

VI. OPTIMIZATION OF THE NUMBER OF JOLT MAPS

We achieved our primary goal of finding a jolt factorization of the map $\mathscr{M}_P$ in the previous section. We now seek to optimize this solution. More specifically, we attempt to reduce the number of jolt maps to a minimum.

We start with the following result from the previous section:

$$f_n=\int_{\mathrm{SU}(3)} du\ g(u)\hat{R}(u)q_1^n, \tag{6.1}$$

where $g(u)$ is given by Eq. (5.17). Here, we take a single jolt monomial q_1^n and act on it with the group SU(3). An alternative procedure is considered below. We will show that it reduces the number of jolt maps required by a substantial amount.

First, we factor SU(3) into the orthogonal group SO(3) and SU(3)/SO(3). The group SO(3) is taken to be the rotation group in the q_1, q_2, q_3 space. We will provide the reason for employing this factorization later. For the sake of notational convenience, let us denote SU(3)/SO(3) by G'. To proceed further, we write u [belonging to the group SU(3)] as the following product of elements belonging to G' and SO(3):

$$u=c\cdot r, \quad u\in\mathrm{SU}(3), \quad c\in G', \quad r\in\mathrm{SO}(3). \tag{6.2}$$

Then, it can be shown[12] that the following relation holds between the measure du for SU(3) and the measures dc and dr for G' and SO(3), respectively:

$$du=dc\cdot dr. \tag{6.3}$$

Substituting these results into the expression for f_n [cf. Eq. (6.1)], we obtain the relation

$$f_n=\int_{G'} dc\int_{\mathrm{SO}(3)} dr\ \ g(c\cdot r)\hat{R}(c\cdot r)q_1^n. \tag{6.4}$$

Letting the SO(3) part of $\hat{R}(c\cdot r)$ act first on q_1^n, we get the following result:

$$\hat{R}(c\cdot r)q_1^n=\hat{R}(c)\sum_{k=1}^{N'(n)} d_k(r)P_k^{(n)}(q_1,q_2,q_3). \tag{6.5}$$

Here we have used the following relation:

$$\hat{R}(r)q_1^n=\sum_{k=1}^{N'(n)} d_k(r)P_k^{(n)}(q_1,q_2,q_3), \quad r\in \mathrm{SO}(3), \tag{6.6}$$

where $P_k^{(n)}(q_1,q_2,q_3)$ denotes a nth degree basis monomial in variables q_1, q_2, and q_3:

$$P_k^{(n)}(q_1,q_2,q_3)=q_1^{n_1}q_2^{n_2}q_3^{n_3}, \quad n_1\geqslant n_2\geqslant n_3,\ \ n_1+n_2+n_3=n. \tag{6.7}$$

The number $N'(n)$ of nth degree basis monomial in three variables is given by the following relation:[7]

$$N'(n)=\binom{n+2}{n}. \tag{6.8}$$

Substituting Eq. (6.5) into Eq. (6.4), we get the relation

$$f_n=\int_{G'} dc\hat{R}(c)\int_{\mathrm{SO}(3)} dr\ g(c\cdot r)\sum_{k=1}^{N'(n)} d_k(r)P_k^{(n)}(q_1,q_2,q_3). \tag{6.9}$$

Next, we define a function $h_k(c)$ by the following relation:

$$h_k(c)\equiv\int_{\mathrm{SO}(3)} dr\ g(c\cdot r)\sum_{k=1}^{N'(n)} d_k(r). \tag{6.10}$$

We have already calculated $g(c\cdot r)$. It is nothing but the function $g(u)$ given in Eq. (5.17). Thus, $h_k(c)$ is well defined and can be calculated. Inserting Eq. (6.10) into Eq. (6.9), we obtain the following result:

$$f_n=\int_{G'} dc\hat{R}(c)\sum_{k=1}^{N'(n)} h_k(c)P_k^{(n)}(q_1,q_2,q_3). \tag{6.11}$$

Next, we need to obtain the discrete version of the above equation. This is again done by going over to a discrete sum over SU(3)/SO(3). Starting from a discrete subgroup of SU(3), one can go over to SU(3)/SO(3) following the procedure outlined in Appendix C. We obtain the following solution:

$$f_n=\int_{G'} dc\hat{R}(c)\sum_{k=1}^{N'(n)} h_k(c)P_k^{(n)}(q_1,q_2,q_3)=\frac{1}{K(G')}\sum_{l=1}^{K(G')}\hat{R}(c_l)\sum_{k=1}^{N'(n)} h_k(c_l)P_k^{(n)}(q_1,q_2,q_3). \tag{6.12}$$

Here, $K(G')$ gives the number of jolt maps required.

We now turn to the task of determining the number of jolt maps $K(G')$. It depends on G' as indicated. We have already seen in Section V that K is determined by looking at the equation for n equal to P (the maximum order). Setting n equal to P in the above expression, we obtain the following result:

$$f_P=\frac{1}{K(G')}\sum_{l=1}^{K(G')}\hat{R}(c_l)\sum_{k=1}^{N'(P)}h_k(c_l)P_k^{(P)}(q_1,q_2,q_3). \tag{6.13}$$

Since the Pth degree homogeneous polynomial f_P on the left hand side has $N(P)$ independent coefficients [cf. Eq. (3.14)], we need $N(P)$ linearly independent vectors on the right hand side. Only then, we can express any f_P in terms of these vectors.

We are now in a position to justify our decision to factor SU(3) into SO(3) and SU(3)/SO(3). Suppose we had not factorized SU(3) as above. Then the analogue of the above equation would be

$$f_P=\frac{1}{K'}\sum_{k=1}^{K'}g(u_i)\hat{R}(u_i)q_1^P, \tag{6.14}$$

where u_i belongs to a discrete subgroup of SU(3). Since we need $N(P)$ independent coefficients to describe f_P, K' has to equal $N(P)$. On the other hand, with factorization we need only $N''(P)$ jolts in Eq. (6.13) where

$$N''(P)=N(P)/N'(P). \tag{6.15}$$

This can be seen as follows. Equation (6.13) can be rewritten to give

$$f_P=\frac{1}{K(G')}\sum_{l=1}^{K(G')}\hat{R}(c_l)H_l(q_1,q_2,q_3), \tag{6.16}$$

where

$$H_l(q_1,q_2,q_3)=\sum_{k=1}^{N'(P)}h_k(c_l)P_k^{(P)}(q_1,q_2,q_3). \tag{6.17}$$

Now, the linear combination of $N'(P)$ jolt polynomials given by $H_l(q_1,q_2,q_3)$ is again a jolt polynomial. Since the jolt polynomial $H_l(q_1,q_2,q_3)$ itself has $N'(P)$ independent coefficients, $K(G')$ needs to be equal only to $N''(P)$ [cf. Eq. (6.15)] in order to give a total of $N(P)$ independent coefficients. On the other hand, in Eq. (6.14), we only have a single jolt monomial q_1^P and hence a single coefficient. Therefore, K' has to equal $N(P)$ in this case.

The above discussion demonstrates that a fewer number of jolts are required when SU(3) is factored into G' and SO(3). We now argue that factorizing SU(3) into a different set of factors does not give an even better result. First, we note that q_1, q_2, q_3 space (or equivalently, p_1, p_2, p_3 space) gives the maximal subspace of commuting jolt polynomials. We cannot choose any group larger than SO(3) since it is shown in Appendix D that SO(3) is the largest subgroup of Sp(6,R) that leaves the q_1, q_2, q_3 space invariant. If we choose a group smaller than SO(3), we will not get all the $N'(P)$ jolt monomials. Then $K(G')$ might have to be larger to get $N(P)$ independent coefficients. Therefore, factoring SU(3) into G' and SO(3) does appear to be the best compromise.

For P equal to 6, $N''(P)$ is equal to 17 from the above procedure [cf. Eqs. (6.15), (3.14) and (6.8)]. From Appendix C, we find that starting from (a similarity transformation of) a discrete subgroup of order 108 of SU(3), one can go over to a set of 18 elements belonging to SU(3)/SO(3). Thus, the number of jolt maps $K(G')$ required for $P=6$ is 18. For this case, we have verified that we do get the required number of linearly independent vectors on the right hand side of Eq. (6.13). Irwin[8] factorizes G as U(1)×U(1)×U(1). Using this factorization, for $P=6$, one needs 27 jolt maps. Thus, we find that the number of jolt maps required in our case is less. When using our factorization for long-term stability analysis of Hamiltonian systems, this can lead to substantial savings in computer time.

VII. SUMMARY

When a nonlinear symplectic map is used in numerical calculations, one is forced to truncate the map at a given order in phase space variables. This truncated map (also known as a symplectic jet) violates the symplectic condition and typically exhibits spurious damping or growth when used to analyze long-term behavior of particle trajectories. We therefore approximated the map by a finite product of symplectic jolt maps which constitutes a symplectic completion of the jet. The action of jolt maps on phase space functions can be evaluated exactly and this should lead to better predictions of long-term stability in complicated Hamiltonian systems. Further, our jolt factorization was optimized so that the number of jolt maps required was significantly reduced. This can result in substantial savings in computer time when used for long-term stability studies. Finally, for $P=6$, we explicitly demonstrated that a fewer number of jolt maps were required as compared to Irwin's procedure.[8] We believe this will be true even for a general P since we are using a bigger group.

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APPENDIX A: EXAMPLES OF JOLT MAPS

Proof of Theorem 1: (i) The equality in Eq. (2.2) follows from Eq. (2.4) and properties of Lie transformations.[9] To show that $e^{:\hat{R}q_1^n:}$ is a jolt map, we start by making the following identification:

$$\exp(:\hat{R}q_1^n:) = \exp(:(\hat{R}q_1)^n:), \tag{A1}$$

where [cf. Eq. (2.4)]

$$\hat{R}q_1 = R_{11}q_1 + R_{12}p_1 + \cdots + R_{16}p_3. \tag{A2}$$

The action of the Lie operator $:(\hat{R}q_1)^n:$ on the phase space variables is given by the relations

$$\begin{aligned} :(\hat{R}q_1)^n:z_i &= -n(\hat{R}q_1)^{n-1}R_{1\,i+1}, \quad i=1,3,5, \\ :(\hat{R}q_1)^n:z_i &= n(\hat{R}q_1)^{n-1}R_{1\,i-1}, \quad i=2,4,6. \end{aligned} \tag{A3}$$

Now, consider the action of $:(\hat{R}q_1)^n:^2$ on the phase space variables. Using Eq. (A3) we obtain the following result:

$$\begin{aligned} :(\hat{R}q_1)^n:^2 z_i &= -nR_{1\,i+1}[(\hat{R}q_1)^n,(\hat{R}q_1)^{n-1}], \quad i=1,3,5, \\ :(\hat{R}q_1)^n:^2 z_i &= nR_{1\,i-1}[(\hat{R}q_1)^n,(\hat{R}q_1)^{n-1}], \quad i=2,4,6. \end{aligned} \tag{A4}$$

But[9]

$$[(\hat{R}q_1)^n,(\hat{R}q_1)^{n-1}] = \hat{R}[q_1^n,q_1^{n-1}] = 0. \tag{A5}$$

This proves that $e^{:\hat{R}q_1^n:}$ is a jolt map.

(ii) We note that the equality in Eq. (2.3) follows from Eq. (2.4) and properties of Lie transformations.[9] We also note that the following equality is satisfied:[9]

$$\hat{R}f(q_1,q_2,q_3)=f(\hat{R}q_1,\hat{R}q_2,\hat{R}q_3). \tag{A6}$$

Consider

$$:\hat{R}f(q_1,q_2,q_3):z_i=[f(\hat{R}q_1,\hat{R}q_2,\hat{R}q_3),z_i]. \tag{A7}$$

Since $\hat{R}q_i$ is linear in the phase space variables, the right hand side can be a function only of $\hat{R}q_i$'s. Denote this function by h. Thus

$$:\hat{R}f(q_1,q_2,q_3):z_i=h(\hat{R}q_1,\hat{R}q_2,\hat{R}q_3)=\hat{R}h(q_1,q_2,q_3), \tag{A8}$$

where the last equality follows from standard properties of Lie transformations.[9]

Next, consider the action of $:\hat{R}f:^2$ on the phase space variables. Using Eq. (A8) we get

$$:\hat{R}f(q_1,q_2,q_3):^2z_i=[\hat{R}f(q_1,q_2,q_3),\hat{R}h(q_1,q_2,q_3)]. \tag{A9}$$

Again using properties of Lie transformations,[9] we obtain

$$:\hat{R}f(q_1,q_2,q_3):^2z_i=\hat{R}[f(q_1,q_2,q_3),h(q_1,q_2,q_3)]. \tag{A10}$$

Since q_i's commute with one another, the Poisson bracket on the right hand side is identically zero. Therefore, $e^{:\hat{R}f(q_1,q_2,q_3):}$ is indeed a jolt map. This completes the proof of the theorem.

APPENDIX B: REPRESENTATIONS OF SU(3) CARRIED BY $q_1^{(n)}$

In this appendix, we prove a theorem regarding the representations of SU(3) carried by the monomial q_1^n. The proof will be a constructive one. Therefore, as a by-product, we obtain the explicit decomposition of q_1^n in terms of the SU(3) basis vectors. We end this appendix with an example. Using the formulas derived during the course of proving the theorem, we decompose q_1^4 in terms of the SU(3) basis vectors.

Let us denote the SU(3) basis vectors by $|j_1,j_2;I,I_3,Y\rangle$. Here j_1 and j_2 label the irreducible representations of SU(3) and I, I_3 and Y label weight vectors within the irreducible representation. It can be shown[13–15] that these basis vectors are associated with harmonic functions on the 5-sphere S^5. The 5-sphere is defined by the relation

$$Z_1^*Z_1+Z_2^*Z_2+Z_3^*Z_3=r^2=1, \tag{B1}$$

where

$$Z_j\equiv\frac{1}{\sqrt{2}}(q_j+ip_j), \tag{B2}$$

$$Z_j^*\equiv\frac{1}{\sqrt{2}}(q_j-ip_j). \tag{B3}$$

Since we are interested in functions defined on the 5-space S^5, it is convenient to parametrize S^5 in terms of polar coordinates ϕ_1, ϕ_2, ϕ_3, θ and ξ. These coordinates are related to the complex phase space variables by the following relations:

$$Z_1 = re^{i\phi_1}\cos\theta, \tag{B4}$$

$$Z_2 = re^{i\phi_2}\sin\theta\cos\xi, \tag{B5}$$

$$Z_3 = re^{i\phi_3}\sin\theta\sin\xi, \tag{B6}$$

where

$$0 \leqslant \phi_1, \phi_2, \phi_3 \leqslant 2\pi; \quad 0 \leqslant \theta, \xi \leqslant \pi/2. \tag{B7}$$

It can be shown[15] that states within the irreducible representation (j_1, j_2) can be associated with harmonic functions defined on S^5 as shown below:

$$|j_1, j_2; I, I_3, Y\rangle = \frac{1}{\sin\theta}\, d^{(1/2)(j_1+j_2+1)}_{(1/6)(j_1-j_2-3Y+6I+3),(1/6)(j_1-j_2-3Y-6I-3)}(2\theta)\, d^{(I)}_{(1/3)(j_1-j_2)+1/2Y, I_3}$$
$$\times(2\xi)\, e^{(1/3)i(j_1-j_2)(\phi_1+\phi_2+\phi_3)} e^{iI_3(\phi_2-\phi_3)} e^{(1/2)iY(-2\phi_1+\phi_2+\phi_3)}. \tag{B8}$$

Here $d^{(j)}_{m',m}(\beta)$ are the usual d-functions that characterize the irreducible representation (j) of SU(2). The sign convention for the d-function is taken to be that given in Edmonds,[16] i.e.,

$$d^{(j)}_{m',m}(\beta) = \langle jm' | \exp(+i\beta J_y/h) | jm\rangle. \tag{B9}$$

where $|jm\rangle$ denotes states within the representation (j) of SU(2).

The d-functions can be computed using the following formula:[17]

$$d^{(j)}_{m',m}(\beta) = [(j+m')!(j-m')!(j+m)!(j-m)!]^{1/2}$$
$$\times \sum_s \frac{(-1)^s \left(\cos\frac{\beta}{2}\right)^{2j+m-m'-2s} \left(\sin\frac{\beta}{2}\right)^{m'-m+2s}}{(j+m-s)!\,s!\,(m'-m+s)!\,(j-m'-s)!}, \tag{B10}$$

where the summation index s ranges over all integral values such that the factorials in the denominator are non-negative. The d-functions can also be computed using the following recursion relation:[17]

$$d^{(j)}_{m',m}(\beta) = \left(\frac{j-m'}{j-m}\right)^{1/2} d^{(j-1/2)}_{m'+1/2,m+1/2}(\beta)\cos\frac{\beta}{2} + \left(\frac{j+m'}{j-m}\right)^{1/2} d^{(j-1/2)}_{m'-1/2,m+1/2}(\beta)\sin\frac{\beta}{2}, \quad \text{if } j \neq m. \tag{B11}$$

If j is equal to m, the following relation can be used:

$$d^{(j)}_{m',j}(\beta) = (-1)^{j-m'} \left[\frac{(2j)!}{(j+m')!(j-m')!}\right]^{1/2} \left(\cos\frac{\beta}{2}\right)^{j+m'} \left(\sin\frac{\beta}{2}\right)^{j-m'}. \tag{B12}$$

Two additional formulas which facilitate computation of the d-functions are given below

$$d^{(j)}_{m',m}(\beta) = (-1)^{m'-m} d^{(j)}_{m,m'}(\beta), \tag{B13}$$

$$d^{(j)}_{m',m}(\beta) = (-1)^{m'-m} d^{(j)}_{-m',-m}(\beta), \tag{B14}$$

We are now in a position to state and prove the theorem on the SU(3) content of q_1^n.

Theorem 2: *The monomial* q_1^n *contains only those representations* (j_1,j_2) *of* SU(3) *for which* j_1+j_2 *is less than or equal to n. Moreover, each such representation occurs once and only once in* q_1^n.

Proof: From Eq. (B4), we obtain the following expression for q_1^n in terms of the coordinates that parametrize the 5-sphere:

$$q_1^n=2^{n/2}(\mathrm{Re}\ Z_1)^n=2^{n/2}r^n\cos^n\phi_1\cos^n\theta. \tag{B15}$$

However, $\cos^n\phi_1$ satisfies the relation[18]

$$\cos^n\phi_1=\sum_{\substack{j_1+j_2=n\\ j_1\geqslant j_2}} a_{j_1j_2}\cos[(j_1-j_2)\phi_1], \tag{B16}$$

where

$$a_{j_1j_2}=\frac{1}{2^{n-1}}\binom{n}{j_2},\quad j_1+j_2=n,\ j_1>j_2, \tag{B17}$$

$$a_{j_1j_2}=\frac{1}{2^{n}}\binom{n}{j_2},\quad j_1+j_2=n,\ j_1=j_2. \tag{B18}$$

Notice that we have denoted the summation indices by j_1 and j_2 in anticipation of results to come. Substituting Eq. (B16) into Eq. (B15), we obtain the result

$$q_1^n=2^{n/2}r^n\sum_{\substack{j_1+j_2=n\\ j_1\geqslant j_2}} a_{j_1j_2}\cos[(j_1-j_2)\phi_1]\cos^{j_1+j_2}\theta. \tag{B19}$$

The above result has to be expressed in terms of the SU(3) state vectors given by $|j_1,j_2;I,I_3,Y\rangle$ [cf. Eq. (B8)]. However, q_1^n does not depend on the coordinates ϕ_2, ϕ_3, and ξ. Therefore, only those SU(3) state vectors that satisfy the following conditions can occur in the expansion of q_1^n:

$$I=I_3=0,\quad Y=-2(j_1-j_2)/3. \tag{B20}$$

Imposing these conditions on a general $|j_1,j_2;I,I_3,Y\rangle$ [cf. Eq. (B8)], we obtain the relation

$$|j_1,j_2;0,0,-2(j_1-j_2)/3\rangle=\frac{1}{\sin\theta}d^{(1/2)(j_1+j_2+1)}_{(1/2)(j_1-j_2+1),(1/2)(j_1-j_2-1)}(2\theta)e^{i(j_1-j_2)\phi_1}. \tag{B21}$$

As expected, these vectors do not depend on the coordinates ϕ_2, ϕ_3, and ξ. The d-function appearing in the above expression satisfies the following property [cf. Eqs. (B13) and (B14)]:

$$d^{(1/2)(j_1+j_2+1)}_{(1/2)(j_1-j_2+1),(1/2)(j_1-j_2-1)}(2\theta)=d^{(1/2)(j_2+j_1+1)}_{(1/2)(j_2-j_1+1),(1/2)(j_2-j_1-1)}(2\theta). \tag{B22}$$

That is, this function is invariant under the exchange of the indices j_1 and j_2. Using this property and Eq. (B21), we obtain the following result:

$$\begin{aligned}&\tfrac{1}{2}[|j_1,j_2;0,0,-2(j_1-j_2)/3\rangle+|j_2,j_1;0,0,-2(j_2-j_1)/3\rangle]\\&\quad=\cos[(j_1-j_2)\phi_1]\frac{1}{\sin\theta}d^{(1/2)(j_1+j_2+1)}_{(1/2)(j_1-j_2+1),(1/2)(j_1-j_2-1)}(2\theta),\quad j_1\geqslant j_2.\end{aligned} \tag{B23}$$

Here we have also used the standard relation

$$\tfrac{1}{2}\,[e^{i(j_1-j_2)\phi_1}+e^{-i(j_1-j_2)\phi_1}]=\cos[(j_1-j_2)\phi_1]. \tag{B24}$$

Comparing Eq. (B23) with the summand on the right hand side of Eq. (B19), we note that we somehow have to generate the function $\cos^{j_1+j_2}\theta$ out of the d-functions by taking appropriate linear combinations. In order to accomplish this, we first need explicit expressions for the d-functions. From Eq. (B10), we get the following result:

$$\begin{aligned}&\frac{1}{\sin\,\theta}\,d^{(1/2)(j_1+j_2+1)}_{(1/2)(j_1-j_2+1),(1/2)(j_1-j_2-1)}(2\theta)\\&=[j_1!(j_1+1)!j_2!(j_2+1)!]^{1/2}\sum_{s=0}^{j_2}\frac{(-1)^s(\cos\,\theta)^{j_1+j_2-2s}(\sin\,\theta)^{2s}}{s!(s+1)!(j_1-s)!(j_2-s)!},\quad j_1\geqslant j_2.\end{aligned} \tag{B25}$$

Using the standard binomial theorem, we obtain the relation

$$(\sin\,\theta)^{2s}=(1-\cos^2\,\theta)^s=\sum_{k=0}^{s}\binom{s}{k}(-1)^{s-k}(\cos^2\,\theta)^{s-k}. \tag{B26}$$

Substituting this relation into Eq. (B25), we get

$$\begin{aligned}&\frac{1}{\sin\,\theta}\,d^{(1/2)(j_1+j_2+1)}_{(1/2)(j_1-j_2+1),(1/2)(j_1-j_2-1)}(2\theta)\\&=[j_1!(j_1+1)!j_2!(j_2+1)!]^{1/2}\sum_{s=0}^{j_2}\frac{1}{s!(s+1)!(j_1-s)!(j_2-s)!}\\&\times\sum_{k=0}^{s}\binom{s}{k}(-1)^k(\cos\,\theta)^{j_1+j_2-2k},\quad j_1\geqslant j_2.\end{aligned} \tag{B27}$$

We had noticed earlier [cf. Eq. (B23)] that the sum of the state vectors $|j_1,j_2;0,0,-2(j_1-j_2)/3\rangle$ and $|j_2,j_1;0,0,-2(j_2-j_1)/3\rangle$ is proportional to $\cos[(j_1-j_2)\phi_1]$ [cf. Eq. (B23)]. This remains true even if we make the following substitution:

$$j_1\rightarrow j_1-i,\quad j_2\rightarrow j_2-i, \tag{B28}$$

where i is some integer. More specifically, we have the following relation:

$$\begin{aligned}&\tfrac{1}{2}\,[|j_1-i,j_2-i;0,0,-2(j_1-j_2)/3\rangle+|j_2-i,j_1-i;0,0,-2(j_2-j_1)/3\rangle]\\&=\frac{1}{\sin\,\theta}\,d^{(1/2)(j_1+j_2+1-2i)}_{(1/2)(j_1-j_2+1),(1/2)(j_1-j_2-1)}(2\theta)\cos[(j_1-j_2)\phi_1],\quad j_1\geqslant j_2,\ i\leqslant j_2,\end{aligned} \tag{B29}$$

where

$$\frac{1}{\sin\theta}\, d^{(1/2)(j_1+j_2+1-2i)}_{(1/2)(j_1-j_2+1),(1/2)(j_1-j_2-1)}(2\theta) = [(j_1-i)!(j_1+1-i)!(j_2-i)!(j_2+1-i)!]^{1/2} \times \sum_{s=0}^{j_2-i} \frac{1}{s!(s+1)!(j_1-s-i)!(j_2-s-i)!} \sum_{k=0}^{s} \binom{s}{k} \times(-1)^k(\cos\theta)^{j_1+j_2-2k-2i}, \quad j_1 \geqslant j_2. \tag{B30}$$

Therefore, the most general combination of vectors that still gives a quantity proportional to $\cos[(j_1-j_2)\phi_1]$ is as follows:

$$2^{n/2}r^n \sum_{i=0}^{j_2} \frac{A_i^{(j_1,j_2)}}{2} [|j_1-i,j_2-i;0,0,-2(j_1-j_2)/3\rangle + |j_2-i,j_1-i;0,0,-2(j_2-j_1)/3\rangle] = 2^{n/2}r^n \cos[(j_1-j_2)\phi_1] \sum_{i=0}^{j_2} A_i^{(j_1,j_2)} \frac{1}{\sin\theta}\, d^{(1/2)(j_1+j_2+1-2i)}_{(1/2)(j_1-j_2+1),(1/2)(j_1-j_2-1)}(2\theta), \quad j_1 \geqslant j_2. \tag{B31}$$

Comparing the right hand side of the above equation with the summand in the expression for q_1^n [cf. Eq. (B19)], we obtain the condition

$$\sum_{i=0}^{j_2} A_i^{(j_1,j_2)} \frac{1}{\sin\theta}\, d^{(1/2)(j_1+j_2+1-2i)}_{(1/2)(j_1-j_2+1),(1/2)(j_1-j_2-1)}(2\theta) = \cos^{j_1+j_2}\theta. \tag{B32}$$

In other words, we need to find coefficients $A_i^{(j_1,j_2)}$ such that the above condition is satisfied. Then, we would have succeeded in decomposing q_1^n in terms of the SU(3) state vectors. We proceed as follows. First, we interchange the summations over indices s and k in Eq. (B30) to obtain the relation

$$\frac{1}{\sin\theta}\, d^{(1/2)(j_1+j_2+1-2i)}_{(1/2)(j_1-j_2+1),(1/2)(j_1-j_2-1)}(2\theta) = B_i^{(j_1,j_2)} \sum_{k=0}^{j_2-i} (-1)^k(\cos\theta)^{j_1+j_2-2k-2i} \times \sum_{s=k}^{j_2-i} \frac{1}{s!(s+1)!(j_1-s-i)!(j_2-s-i)!} \binom{s}{k}, \quad j_1 \geqslant j_2,\ i \leqslant j_2, \tag{B33}$$

where

$$B_i^{(j_1,j_2)} = [(j_1-i)!(j_1+1-i)!(j_2-i)!(j_2+1-i)!]^{1/2}. \tag{B34}$$

Inserting Eq. (B33) into Eq. (B32), we get the condition

$$\sum_{i=0}^{j_2} A_i^{(j_1,j_2)} B_i^{(j_1,j_2)} \sum_{k=0}^{j_2-i} (-1)^k(\cos\theta)^{j_1+j_2-2k-2i} \times \sum_{s=k}^{j_2-i} \frac{1}{s!(s+1)!(j_1-s-i)!(j_2-s-i)!} \binom{s}{k} = \cos^{j_1+j_2}\theta, \quad j_1 \geqslant j_2. \tag{B35}$$

The coefficient $C_l^{(j_1,j_2)}$ of $\cos^{j_1+j_2-2l}\theta$ on the left hand side of the above equation is given by the expression (where $l=i+k$)

$$C_l^{(j_1,j_2)}=\sum_{k=0}^{l}(-1)^k A_{l-k}^{(j_1,j_2)}B_{l-k}^{(j_1,j_2)} \times\sum_{s=k}^{j_2-l+k}\frac{1}{s!(s+1)!(j_1-s-l+k)!(j_2-s-l+k)!}\binom{s}{k}, \quad j_1\geqslant j_2. \tag{B36}$$

The above expression can be simplified by using the following substitution

$$s'=s-k. \tag{B37}$$

Making this substitution in Eq. (B36), we get the relation

$$C_l^{(j_1,j_2)}=\sum_{k=0}^{l}\frac{(-1)^k}{k!}A_{l-k}^{(j_1,j_2)}B_{l-k}^{(j_1,j_2)}\sum_{s'=0}^{j_2-l}\frac{1}{s'!(s'+k+1)!(j_1-s'-l)!(j_2-s'-l)!}, \quad j_1\geqslant j_2. \tag{B38}$$

In order to satisfy Eq. (B35), we need to impose the following conditions

$$C_0^{(j_1,j_2)}=1, \tag{B39}$$

$$C_l^{(j_1,j_2)}=0, \quad l=1,2,\ldots,j_2. \tag{B40}$$

Inserting the expression for $C_l^{(j_1,j_2)}$ into the above equations, we obtain the following results:

$$A_0^{(j_1,j_2)}=\frac{1}{B_0^{(j_1,j_2)}S_{00}^{(j_1,j_2)}},$$

$$A_l^{(j_1,j_2)}=\frac{1}{B_l^{(j_1,j_2)}S_{l0}^{(j_1,j_2)}}\sum_{k=1}^{l}\frac{(-1)^{k+1}}{k!}A_{l-k}^{(j_1,j_2)}B_{l-k}^{(j_1,j_2)}S_{lk}^{(j_1,j_2)}, \quad 1\leqslant l\leqslant j_2, \tag{B41}$$

where

$$S_{lk}^{(j_1,j_2)}=\sum_{s'=0}^{j_2-l}\frac{1}{s'!(s'+k+1)!(j_1-s'-l)!(j_2-s'-l)!}. \tag{B42}$$

From Eqs. (B19), (B31), and (B32), we finally get the following decomposition for q_1^n:

$$q_1^n=2^{n/2}r^n\sum_{\substack{j_1+j_2=n\\ j_1\geqslant j_2}}\frac{a_{j_1j_2}}{2} \times\sum_{i=0}^{j_2}A_i^{(j_1,j_2)}[|j_1-i,j_2-i;0,0,-2(j_1-j_2)/3\rangle+|j_2-i,j_1-i;0,0,-2(j_2-j_1)/3\rangle]. \tag{B43}$$

We note that all representations (j_1,j_2) (with j_1+j_2 less than or equal to n) appear in the decomposition (since the coefficients $A_i^{(j_1,j_2)}a_{j_1j_2}$ are seen to be nonzero for all valid j_1, j_2, and i). Furthermore, from each representation (j_1,j_2), only one vector $|j_1,j_2;0,0,-2(j_1-j_2)/3\rangle$ appears in the decomposition. This proves the theorem.

As an example, we obtain the decomposition of q_1^4. Using the above formulas we get the following results:

$$a_{40}=1/8, \quad a_{31}=1/2, \quad a_{22}=3/8; \tag{B44}$$

$$A_0^{(4,0)}=1/\sqrt{5}, \quad A_0^{(3,1)}=1/5\sqrt{2}, \quad A_1^{(3,1)}=\sqrt{3}/5; \tag{B45}$$

$$A_0^{(2,2)}=1/10, \quad A_1^{(2,2)}=4/15, \quad A_2^{(2,2)}=1/6. \tag{B46}$$

Substituting these results into Eq. (B43), we obtain the following decomposition

$$\begin{aligned} q_1^4=&\frac{r^4}{4\sqrt{5}}[|4,0;0,0,-8/3\rangle+|0,4;0,0,8/3\rangle]+\frac{r^4}{5\sqrt{2}}[|3,1;0,0,-4/3\rangle+|1,3;0,0,4/3\rangle] \\ &+\frac{\sqrt{3}r^4}{5}[|2,0;0,0,-4/3\rangle+|0,2;0,0,4/3\rangle]+\frac{3}{20}r^4|2,2;0,0,0\rangle+\frac{2}{5}r^4|1,1;0,0,0\rangle \\ &+\frac{1}{4}r^4|0,0;0,0,0\rangle. \end{aligned} \tag{B47}$$

APPENDIX C: DISCRETE SUBGROUPS OF SU(3)

In this appendix, we study the discrete subgroups of SU(3) which are required in Sections V and VI. We start by defining the following matrices:

$$A(\alpha,\beta)=\begin{pmatrix} e^{i\alpha} & 0 & 0 \\ 0 & e^{i\beta} & 0 \\ 0 & 0 & e^{-i(\alpha+\beta)} \end{pmatrix}, \tag{C1}$$

$$B(\alpha,\beta)=\begin{pmatrix} e^{i\alpha} & 0 & 0 \\ 0 & 0 & e^{i\beta} \\ 0 & e^{i(\pi-\alpha-\beta)} & 0 \end{pmatrix}, \tag{C2}$$

$$E(\alpha,\beta)=\begin{pmatrix} 0 & e^{i\alpha} & 0 \\ 0 & 0 & e^{i\beta} \\ e^{-i(\alpha+\beta)} & 0 & 0 \end{pmatrix}, \tag{C3}$$

$$V=\frac{1}{\sqrt{3}i}\begin{pmatrix} 1 & 1 & 1 \\ 1 & \omega & \omega^2 \\ 1 & \omega^2 & \omega \end{pmatrix}, \tag{C4}$$

$$V'=\frac{1}{\sqrt{3}i}\begin{pmatrix} 1 & 1 & \omega^2 \\ 1 & \omega & \omega \\ \omega & 1 & \omega \end{pmatrix}, \tag{C5}$$

$$W=\frac{1}{2}\begin{pmatrix} -1 & \mu_2 & \mu_1 \\ \mu_2 & \mu_1 & -1 \\ \mu_1 & -1 & \mu_2 \end{pmatrix}, \tag{C6}$$

$$Z=\frac{-1}{\sqrt{7}i}\begin{pmatrix} a & b & c \\ b & c & a \\ c & a & b \end{pmatrix}, \tag{C7}$$

where

$$\omega=e^{i2\pi/3}, \tag{C8}$$

$$\mu_1=\tfrac{1}{2}(-1+\sqrt{5}), \quad \mu_2=\tfrac{1}{2}(-1-\sqrt{5}), \tag{C9}$$

$$a=\xi^4-\xi^3, \quad b=\xi^2-\xi^5, \tag{C10}$$

$$c=\xi-\xi^6, \quad \xi^7=1. \tag{C11}$$

The discrete subgroups of SU(3) are listed below along with their generators.[19,20] First, we list the crystal-like subgroups. They are denoted by $\Gamma(n)$ where n denotes the order of the group:

(1) $\Gamma(60){:}A(0,\pi)$, $E(0,0)$, and W;
(2) $\Gamma(108){:}A(0,2\pi/3)$, $E(0,0)$, and V;
(3) $\Gamma(168){:}A(2\pi/7,4\pi/7)$, $E(0,0)$, and Z;
(4) $\Gamma(216){:}A(0,2\pi/3)$, $E(0,0)$, V, and V';
(5) $\Gamma(648){:}A(0,2\pi/3)$, $E(0,0)$, V, and $A(4\pi/9,4\pi/9)$;
(6) $\Gamma(1080){:}A(0,\pi)$, $E(0,0)$, W, and $B(\pi,5\pi/3)$.

Next, we list the dihedral-like groups and the disconnected groups. They are denoted by $\Delta(n)$ where n denotes the order of the group:

(1) $\Delta(3m^2){:}A(j2\pi/m,k2\pi/m)$ and $E(0,0)$ where j and k are integers;
(2) $\Delta(6m^2){:}A(j2\pi/m,k2\pi/m)$, $E(0,0)$, and $B(j2\pi/m,k2\pi/m)$ where j and k are integers;
(3) $\Delta(3\infty^2){:}A(\alpha,\beta)$ and $E(0,0)$;
(4) $\Delta(6\infty^2){:}A(\alpha,\beta)$, $E(0,0)$, and $B(\alpha,\beta)$.

In Section VI, we will also be interested in discrete elements of SU(3)/SO(3). We obtain discrete elements of SU(3)/SO(3) by the following procedure. We start with a discrete subgroup $\Gamma(n)$ of SU(3). Next, we identify the subgroup $\Gamma'(n')$ of $\Gamma(n)$ that belongs to SO(3) [where n' is the order of $\Gamma'(n')$]. This is easily accomplished once it is realized that an element $\Gamma_i\in\Gamma(n)$ belongs to SO(3) if and only if all its matrix elements are real. For example, it is seen that all of $\Gamma(60)$ also belongs to SO(3) since each of its elements is real. Next, we construct the $\Gamma(n)/\Gamma'(n')$ as follows. For every element Γ_i belonging to $\Gamma(n)$, we form the right coset $\Gamma'(n')\Gamma_i$. There will be n/n' distinct right cosets. From each distinct coset, we select one element to be the coset representative. These n/n' coset representatives belong to $\Gamma(n)/\Gamma'(n')$. Thus we get a collection of n/n' discrete elements of SU(3)/SO(3). Values for n' and n/n' for the various crystal groups are given below:

(1) $\Gamma(60){:}n'=60$, $n/n'=1$;
(2) $\Gamma(108){:}n'=6$, $n/n'=18$;
(3) $\Gamma(168){:}n'=6$, $n/n'=28$;
(4) $\Gamma(216){:}n'=6$, $n/n'=36$;

(5) $\Gamma(648){:}n'=6,\ n/n'=108$;
(6) $\Gamma(1080){:}n'=60,\ n/n'=18$.

Finally, we should mention that we rarely make direct use of the complex 3×3 matrices Γ_i belonging to $\Gamma(n)$. We need objects that act on the six dimensional phase space. Therefore, we first embed these complex 3×3 matrices into the compact part of Sp(6,R) following the procedure outlined in Appendix D. The real 6×6 matrices that are obtained as a result of this embedding (and the Lie transformations corresponding to these matrices) can act on phase space variables. It is these real 6×6 matrices that are used in Sections V and VI.

APPENDIX D: LARGEST SUBGROUP OF SU(3) THAT LEAVES COORDINATE SPACE INVARIANT

In this appendix, we prove a theorem satisfied by the special orthogonal group SO(3). The result of this theorem will be used in Section VI. Throughout this appendix, we will work in the rearranged basis of phase space variables given by $z=(q_1,q_2,q_3,p_1,p_2,p_3)$ for convenience. Symplectic matrices in the rearranged basis are related to those in the original basis by a simple similarity transformation.

Theorem 3: *Let $V^{(m)}$ be the vector space formed by homogeneous polynomials of degree m in variables q_1, q_2, and q_3. Then,* SO(3) *is the largest subgroup of* SU(3) *that leaves $V^{(m)}$ invariant.*

Proof: We first prove the following lemma.

Lemma 1: SO(3) *is the largest subgroup of* SU(3) *that leaves $V^{(1)}$ invariant.*

Proof: Consider a complex 3×3 matrix R belonging to SU(3). It satisfies the following conditions:

$$R^{\dagger}=R^{-1};\quad \det R=1. \tag{D1}$$

It can be decomposed into its real and imaginary parts as follows

$$R=-D+iC, \tag{D2}$$

where C and D are real 3×3 matrices.

Since the matrix R has to act on functions of phase space variables, we first need to embed it in the compact part of Sp(6,R). Following the procedure outlined in Ref. 7, the real 6×6 symplectic matrix U^s (in the rearranged basis) corresponding to the unitary matrix R is given by the relation

$$U^s=V^s\begin{pmatrix} R & 0\\ 0 & R^* \end{pmatrix}(V^s)^{-1}, \tag{D3}$$

where V^s is given by[9]

$$V^s=\frac{1}{\sqrt{2}}\begin{pmatrix} I & iI\\ iI & I \end{pmatrix}. \tag{D4}$$

Here I is a 3×3 identity matrix. Upon evaluating this equation, we obtain the following result:

$$U^s=\begin{pmatrix} -D & C\\ -C & -D \end{pmatrix}. \tag{D5}$$

Next, consider a general 6-vector v^s belonging to $V^{(1)}$. It is given by the relation

$$v^s=(v_3^s,0_3) \tag{D6}$$

where v_3^s and 0_3 are 3-vectors defined as follows:

$$v_3^s=(a,b,c), \quad a,b,c\in\mathscr{R} \tag{D7}$$

$$0_3=(0,0,0). \tag{D8}$$

The action of U^s on v^s is given by the following relation:

$$U^s v^s=\begin{pmatrix} -Dv_3^s \\ -Cv_3^s \end{pmatrix}. \tag{D9}$$

Therefore, $U^s v^s$ belongs to $V^{(1)}$ if and only if the following condition is satisfied [cf. Eq. (D6)]

$$Cv_3^s=0. \tag{D10}$$

Since v_3^s is an arbitrary 3-vector, this implies that C is a zero matrix:

$$C=0. \tag{D11}$$

Substituting Eq. (D11) into Eq. (D5), the most general element belonging to the compact part of Sp(6,R) that leaves $V^{(1)}$ invariant is found to have the following form:

$$U_*^s=\begin{pmatrix} -D & 0 \\ 0 & -D \end{pmatrix}. \tag{D12}$$

We convert this into an element of SU(3) using the following procedure.[8] Given a 6×6 matrix U^s belonging to the compact part of Sp(6,R), one can extract the complex 3×3 matrix R belonging to SU(3) from it through the following relation:

$$(V^s)^{-1}U^sV^s=\begin{pmatrix} R & 0 \\ 0 & R^* \end{pmatrix}. \tag{D13}$$

From the above equation, we obtain the SU(3) element R_* corresponding to U_*^s as

$$R_*=-D. \tag{D14}$$

However, since this is supposed to be an element of SU(3), it has to satisfy the conditions given in Eq. (D1). Imposing these conditions on R_* and noting that R_* is real, we obtain the following restrictions on R_*:

$$\widetilde{R}_*=R_*^{-1}; \quad \det R_*=1, \tag{D15}$$

where $\widetilde{R}_*$ is the transpose of R_*. But these are precisely the conditions satisfied by an element of SO(3). This proves the lemma.

We now return to the proof of the theorem. Consider an element $P_k^{(m)}$ belonging to $V^{(m)}$:

$$P_k^{(m)}=a_1q_1^m+a_2q_1^{m-1}q_2+\cdots+a_Nq_3^m, \tag{D16}$$

where [cf. Eq. (6.8)]

$$N=\binom{m+2}{m}. \tag{D17}$$

The action of $\hat{U}^s$ (the Lie transformation corresponding to the matrix U^s) on $P_k^{(m)}$ is given as follows:

$$\hat{U}^s P_k^{(m)} = a_1(\hat{U}^s q_1)^m + a_2(\hat{U}^s q_1)^{m-1}(\hat{U}^s q_2) + \cdots + a_N(\hat{U}^s q_3)^m. \tag{D18}$$

Therefore, the condition that ''U^s leaves $V^{(1)}$ invariant'' is sufficient to ensure that $\hat{U}^s$ leaves $V^{(m)}$ invariant, i.e.,

$$\hat{U}^s V^{(1)} \subseteq V^{(1)} \Rightarrow \hat{U}^s V^{(m)} \subseteq V^{(m)}. \tag{D19}$$

To complete the proof of the theorem, we need to show that this is also a necessary condition.

Suppose that $\hat{U}^s V^{(1)} \nsubseteq V^{(1)}$. Then, there exists a vector v_*^s belonging to $V^{(1)}$ that is mapped out of $V^{(1)}$ under the action of $\hat{U}^s$, i.e.,

$$\hat{U}^s v_*^s \notin V^{(1)}. \tag{D20}$$

This can be rewritten as follows

$$\hat{U}^s (\hat{U}_1^s)^{-1} \hat{U}_1^s v_*^s \notin V^{(1)}, \tag{D21}$$

where $\hat{U}_1^s$ is chosen to satisfy the condition

$$\hat{U}_1^s v_*^s = q_1. \tag{D22}$$

This is always possible since v_*^s is effectively a vector in the three dimensional $q_1 - q_2 - q_3$ space and therefore can be rotated to orient it along the q_1 axis. Since the transformation $\hat{U}_1^s$ that brings about this rotation belongs to the subgroup SO(3), $\hat{U}^s(\hat{U}_1^s)^{-1}$ (or more accurately, the unitary matrix corresponding to this transformation) still belongs to SU(3). In summary, if $\hat{U}^s V^{(1)} \nsubseteq V^{(1)}$, there exists a transformation $\hat{U}_2^s$ [equal to $\hat{U}^s(\hat{U}_1^s)^{-1}$] that maps q_1 out of $V^{(1)}$:

$$\hat{U}_2^s q_1 \notin V^{(1)}. \tag{D23}$$

Now, consider the action of $\hat{U}_2^s$ on the vector q_1^m belonging to $V^{(m)}$:

$$\hat{U}_2^s q_1^m = (\hat{U}_2^s q_1)^m. \tag{D24}$$

Since $\hat{U}_2^s q_1$ does not belong to $V^{(1)}$, it will consist of at least one nonzero term containing p_1, p_2, or p_3. Consequently, from the above equation, even $\hat{U}_2^s q_1^m$ will contain at least one such term. Therefore, the following equation is seen to be true:

$$\hat{U}_2^s q_1^m \notin V^{(m)}. \tag{D25}$$

Since we have produced one vector which leaves $V^{(m)}$ under the action of $\hat{U}_2^s$, we have succeeded in proving the following statement:

$$\hat{U}^s V^{(1)} \nsubseteq V^{(1)} \Rightarrow \hat{U}^s V^{(m)} \nsubseteq V^{(m)}. \tag{D26}$$

Combining Eqs. (D19) and (D26), we see that the condition ''$\hat{U}^s$ leaves $V^{(1)}$ invariant'' is both necessary and sufficient to ensure that $\hat{U}^s$ leaves $V^{(m)}$ invariant. Since SO(3) is the largest subgroup of SU(3) satisfying the first condition, it is also the largest subgroup of SU(3) that leaves $V^{(m)}$ invariant. This completes the proof of the theorem.

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