Constructing Dynamical Symmetries

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Abstract

Optical excitation in the dipole approximation and other probes couple two quantum states of an unaddressed finite quantum mechanical discrete system. Thereby the interaction of the system with the probe is bilinear in the coherence between the two states and in the time-dependent strength of the probe. The total Hamiltonian is a sum of such bilinear terms and of terms linear in the populations. The terms in the Hamiltonian form a basis for a Lie algebra that can be represented as a direct product of individual two state systems each using the population and the coherence between two states. Dynamical symmetries can be used to advantage to describe the progress of such systems in time. They also offer a compact and efficient representation for a density matrix of maximal entropy that evolves in time. Using the factorization approach of Wei and Norman, (J. Wei and E. Norman, Lie Algebraic Solution of Linear Differential Equations, J. Math. Phys. **4**, 575 (1963)), we construct a unitary quantum mechanical evolution operator that is a factored contribution of individual two state systems. Thereby one can propagate, to all orders in perturbation theory, both the wave function and the density matrix with special reference to dynamical symmetries.

Significance statement

Dynamical symmetries, time-dependent operators that almost commute with the Hamiltonian, extend the role of ordinary symmetries. They also provide an interesting insight on constants of the motion. Motivated by progress in quantum technologies we illustrate a practical algebraic approach to computing such time-dependent operators. Explicitly we expand them as a linear combination of time-independent operators with time-dependent coefficients. There are possible applications to determining quantum mechanical distributions of maximal entropy and to the dynamics of systems of coherently coupled coherent two state systems, realizable by optical excitation. This formulation generates an Ising-like Hamiltonian where each 'spin' is a state of the unaddressed, free, system and is of potential relevance to quantum computing based on qubit architecture.

Introduction

The dual role of operators that commute with the Hamiltonian as symmetries and as constants of the motion was established very early in quantum mechanics. The application of symmetry was developed in detail as 'group theory' and it became a central component in the bag of tools of chemists, see, e.g., (1) . It was only in the sixties of the previous century that the notion of symmetry was extended to groups of operators that do not necessarily commute with the Hamiltonian. As far as we know there were at the time two main lines of independent and unrelated developments. In retrospect these developments are closely related and in this paper we will take advantage of both. The first development is primarily of mathematical nature. It is to seek analytical solutions of exponential forms of linear differential equations of the first order. The time dependent Schrödinger equation is an equation of this type, as are other well-known equations of mathematical physics, (e.g., the diffusion equation, the master equation). Among these equations the Schrödinger equation is almost unique in that it describes reversible dynamics. A rigorous exponential type solution was presented by Magnus (2) An early application of this work in physicochemical dynamics is by Pechukas and Light (3) and a detailed review of the earlier work is by Wilcox (4) . An early application in optics was by Hioe and Eberly(5) . See also Dattoli (6) and Altafini(7) . Below we use a complementary early mathematical representation of the exponential by Norman and Wei (8, 9) . See also (10) . Beginning in pure mathematics there was also a more general approach that sought to identify symmetries of more general differential equations (11, 12) The work of Wulfman with special reference to time dilation, as summarized in his book (13) is perhaps the best known application in chemical physics. The second development was motivated by the physics of elementary particles. The notion of a dynamical symmetry was introduced there and a detailed review is by Bohm, Ne'eman and Barutc(14) An early application of this concept in scattering theory is by Alhassid and Levine (15) , see also (16) . An early overview is (17) . It was also shown(18) that by elevating time to the role of a dynamical variables, the dynamical symmetries become stationary constants of the motion. Anharmonic systems are treated in ref (19) .

Our intention in this paper is to report on the actual explicit construction of dynamical symmetries. But to motivate some key aspects of this development we need to review yet another theoretical development, the maximum entropy formalism (20, 21) . We do not mean the well-known applications of this formalism to statistical mechanics of equilibrium that started with Gibbs(22) and was brought to the forefront by Jaynes(23) using the axiomatic introduction of entropy from information theory. We discuss in some detail and use the approach of maximum entropy to solve the differential equations of quantum dynamics. There is also the converse, see (24) , where linear time dependent quantum mechanical equations of motion, that can be dissipative, are derived using the maximum entropy formalism.

Explicitly, we seek to construct dynamical symmetries because we intend to use them as the constraints that are imposed in the maximum entropy formalism. The two papers (16) and (15) and the variational formulation of (25) show that the dynamical symmetries imposed as constraints in the process of seeking a maximum of the entropy can generate exact solutions and are equally useful to generate approximations. We discuss this aspect as part of our introduction. Specifically, we want to generate a description of the state of a system that is not stationary but is evolving under the action of a Hamiltonian. The initial state can be either a pure state or a mixture and so one needs to describe the system by a density operator $\rho(t)$ at the time *t*. $\rho(t)$ evolves in time according to the well-known Liouville-von Neumann equation, $\partial\rho/\partial t = [H, \rho]$ where H is the Hamiltonian and we took $\hbar = 1$. The formal solution is $\rho(t) = U(t)\rho(0)U^{\dagger}(t)$ and to make use of it we need to specify an initial state, $\rho(0)$, for the first order equation of motion. $U(t)$ is the unitary evolution operator $i\,\partial U(t)/\partial t = HU(t)$ with the initial condition $U(0) = I$ where *I* is the identity operator. An exponential type solution of this equation for a time dependent Hamiltonian H is one of the key problems that we will address below. Furthermore we want an explicit solution for the unfolding in time of the density operator. In the introduction we proceed with the central need to construct an initial density operator.

From now on in this paper we take it that a practical procedure is typically limited to a Hilbert space that is of a finite dimension, *N*. The dimension can be large but finite. It follows that for our purpose an operator can be represented as an N by N matrix. We need the initial density matrix to be stationary so that it will only change in time due to the action of the Hamiltonian. Our first trivial but useful point is that a stationary N by N density matrix can always be written as a density matrix of maximal entropy subject to N^2 (or, quite often, fewer) time independent Hermitian operators. Motivation: Let $|i\rangle, |j\rangle$ for $i, j \in \{1, \dots, N\}$, be the N basis states in which the matrix $\boldsymbol{\rho}(0)$ is written. Then the diagonal elements, the populations, are specified by the given mean values of the N states $|i\rangle\langle i|$, explicitly these are $\left(\boldsymbol{\rho}(0)\right)_{ii} = Tr(\boldsymbol{\rho}(0)|i\rangle\langle i|)$. The coherences are specified by the $N(N-1)/2$ complex numbers $Tr(\boldsymbol{\rho}(0)|i\rangle\langle j|)$ that are pairwise conjugate to one another, that is by $N(N-1)$ real numbers. These operators are the generators of the Lie algebra $U(N)$. In an advanced text they will be called the Cartan-Weyl basis for that algebra. If we separately require that the density matrix is normalized then we need a total of only additional $N^2 - 1$ constraints and the algebra will be $SU(N)$. In practice we will often need far fewer constraints. A very simple example is if the normalized initial state has an equilibrium thermal distribution with the Hamiltonian H_0. Then we need only two constraints in order to reproduce the initial density matrix namely given normalization $Tr(\boldsymbol{\rho}(0)\boldsymbol{I})$, where $\boldsymbol{I}$ is the identity matrix, and given mean energy, $Tr(\boldsymbol{\rho}(0)\boldsymbol{H}_0)$. The resulting density matrix of maximal entropy is the well-known exponential form $\boldsymbol{\rho}(0) = \exp(-\lambda_0 \boldsymbol{I} - \beta \boldsymbol{H}_0)$. The two parameters λ_0 and β are the Lagrange multipliers imposed in seeking a density matrix of maximal entropy subject to the two constraints. The numerical values of the two Lagrange multipliers are determined by the two expectation values above. Such a density matrix will correctly reproduce the values of all the coherences, namely zero and the mean values of all the populations, namely a Boltzmann distribution. In the more general case, besides normalization there can be more than one constraint needed to specify the initial state $\{\boldsymbol{A}_r\}$, $r = 0,1,2, \ldots$ and $\boldsymbol{A}_0 = \boldsymbol{I}$. The matrices $\boldsymbol{A}_r$ need not commute with one another but in general we expect them to be members of a Lie algebra. Given a set of constraints that are necessary to specify the initial state we enlarge the set, if necessary, so that we have a closed Lie algebra. Since we take it that the Hilbert space is of finite dimensions this is possible. One can transform amongst the members of the set such that the particular choice is not unique, but the algebra is.

A density of maximal entropy that describes the initial state, which is subject to the given set of N^2 or fewer expectation values of the constraints, is of exponential form $\boldsymbol{\rho}(0) = \exp(-\sum_{r=0} \lambda_r \boldsymbol{A}_r)$. The values of the Lagrange multipliers $\{\lambda_r\}$ are determined by the given values of the constraints. Some of these values can be zero. A constraint for which its conjugate Lagrange multiplier has the value zero does not lower the value of the entropy from the maximum as determined by imposing the other constraints. The value of the Lagrange multiplier for a constraint that is not imposed can always be taken as zero. The operators A_r need not commute with one another so care must be exercised in expanding the exponential. But one can show, see (26) for a very careful discussion, that at the maximal entropy the density matrix $\boldsymbol{\rho}(0)$ and the surprisal matrix $\mathfrak{I} \equiv \ln(\boldsymbol{\rho}(0))$ commute.

Dynamical symmetries

Dynamical symmetries, $\boldsymbol{\mathcal{A}}_r(t)$, defined as

$$\partial \boldsymbol{\mathcal{A}}_r(t)/\partial t - [\boldsymbol{H}, \boldsymbol{\mathcal{A}}_r(t)] = 0 \qquad (1)$$

with the initial condition, $\boldsymbol{\mathcal{A}}_r(0) = \boldsymbol{A}_r$ ($\boldsymbol{A}_r$ is a constraint), enter immediately when an initial state of maximal entropy is propagated forward in time with a unitary evolution operator

$$\boldsymbol{\mathcal{A}}_r(t) = \boldsymbol{U}(t)\boldsymbol{A}_r\boldsymbol{U}^\dagger(t) \qquad (2)$$

The time dependent dynamical symmetries enter as the constraints on the density matrix of maximal entropy at the time *t* given an initial density matrix of maximal entropy subject to time independent constraints.

$$\boldsymbol{\rho}(t) = \boldsymbol{U}(t)\boldsymbol{\rho}(0)\boldsymbol{U}^{\dagger}(t) = \boldsymbol{U}(t)\exp(-\textstyle\sum_{r=0}\lambda_r\boldsymbol{A}_r)\boldsymbol{U}^{\dagger}(t) =$$
$$= \exp\left(-\boldsymbol{U}(t)(\textstyle\sum_{r=0}\lambda_r\boldsymbol{A}_r)\,\boldsymbol{U}^{\dagger}(t)\right) = \exp(-\textstyle\sum_{r=0}\lambda_r\boldsymbol{\mathcal{A}}_r(t)).$$

The Lagrange multipliers λ_r conjugate to the dynamical symmetries and retain their initial value. This is to be expected because the mean values of the dynamical symmetries ($\equiv$ constraints) do *not* depend on time

$$Tr\big(\boldsymbol{\rho}(t)\boldsymbol{\mathcal{A}}_r(t)\big) = Tr(\boldsymbol{\rho}(t)\boldsymbol{U}(t)\boldsymbol{A}_r\boldsymbol{U}^{\dagger}(t)) = Tr(\boldsymbol{U}^{\dagger}(t)\boldsymbol{\rho}(t)\boldsymbol{U}(t)\boldsymbol{A}_r) = Tr(\boldsymbol{\rho}(0)\boldsymbol{A}_r) \quad (3)$$

In other words, the time dependent *dynamical symmetries are constants of the motion*. Their expectation value is constant in time. Similarly, the entropy itself remains a constant of motion for the reversible evolution described by a unitary evolution operator. If the Hamiltonian H is time independent than one readily verifies by differentiating equation (2) that if $\boldsymbol{\mathcal{A}}_r(t)$ is a dynamical symmetry then so is its time derivative, $\partial\boldsymbol{\mathcal{A}}_r(t)/\partial t$. It then follows from the Jacobi identity that the set of dynamical symmetries closes a Lie algebra.

A possible intuitive way of accepting that the dynamical operators have expectation values that do not change with time is to recognize that the equation of motion (1) or its formal solution $\boldsymbol{\mathcal{A}}_r(t) = \boldsymbol{U}(t)\boldsymbol{A}_r\boldsymbol{U}^{\dagger}(t)$ corresponds to a Heisenberg picture but with the unusual feature that it is an evolution *backwards* in time. So in equation (3), when the density matrix is moving forward in time while the dynamical symmetry is moving backwards, the product is stationary.

For a system of N states, where N can be quite large but finite, the density matrix of equation (3) is an N by N matrix. It is an exponential function of the Surprisal, $\boldsymbol{\mathfrak{I}}$, a Hermitian N by N matrix. We wish to make a mathematically trivial but a useful comment. A matrix element of an exponential of a matrix will typically *not* look like a single exponential. Rather, since the matrix has N real eigenvalues, the matrix element of the exponential will be a sum of no more than N terms. Indeed, fewer than N terms if some eigenvalues are degenerate. For the simpler case of N distinct eigenvalues of the Surprisal matrix $\boldsymbol{\mathfrak{I}}$ we have a spectral expansion(27)

$$\boldsymbol{\rho} \equiv \exp(-\boldsymbol{\mathfrak{I}}) = \textstyle\sum_{i=1}^{N}\exp\,(-\mathcal{I}_i)\boldsymbol{P_i} \quad (4)$$

where *i* is an index of the eigenvalues $\mathcal{I}_i$, $\boldsymbol{\mathfrak{I}}\boldsymbol{X}_i = \mathcal{I}_i\boldsymbol{X}_i$ and the Hermitian matrices $\boldsymbol{P}_{\mathrm{i}}$ are the projection matrices on the eigenvectors of $\mathfrak{I}$. For a Hermitian matrix $\boldsymbol{P}_i = \boldsymbol{X}_i\boldsymbol{X}_i^{\dagger}$.

In the mathematical literature mentioned in the introduction it is typically assumed that the Hamiltonian $\boldsymbol{H}$ itself is in the algebra and that it can be time dependent in the form

$$\boldsymbol{H} = \sum_r h_r(t)\boldsymbol{A}_r \quad (5)$$

The operators $\boldsymbol{A}_\mathrm{r}$ are members of a Lie algebra and the time dependent coefficients are real or complex as needed so that the Hamiltonian is Hermitian. For this special form the dynamical symmetries can be expressed as linear combinations of the operators of the algebra

$$\boldsymbol{\mathcal{A}}_r(\mathrm{t}) = \sum_s a_{rs}(t)\boldsymbol{A}_s \quad (6)$$

We have finally reached our first point. One central aim of this paper is to determine the time dependent coefficients $a_{rs}(t)$ in a systematic manner, preferably particularly suited to a quantum computer that is built as a set of coupled qubits.

The linear expansion, equation (6), for the dynamical symmetries means that one can introduce time dependent Lagrange multipliers $\{\lambda_r(t)\}$ that are conjugate to the time independent constraints $\{\boldsymbol{A}_r\}$. From the two ways of writing the surprisal $\sum_r \lambda_r \boldsymbol{\mathcal{A}}_r(\mathrm{t}) = \sum_s \lambda_s(t)\mathbf{A}_s$ and the orthogonality of the constraints and equation (6) it follows that the Lagrange multipliers evolve in time in an opposite, contragradient, way to the constraints

$$\sum_r \lambda_r\, a_{rs}(t) = \lambda_s(t)$$

One can be concerned that the assumption about the linear structure of the Hamiltonian, equation (5), is too restrictive. Actually, not quite. In any realistic application we will work in an enumerable, N dimensional Hilbert space. Then there is a Cartan-Weyl type basis for $U(N)$ as discussed above. It can well be that a smaller algebra is enough but with N^2 operators we can take a system of N states that are pairwise coupled and write the Hamiltonian as a linear sum over N^2 terms, $H = \sum_{i,j} H_{ij}\, |i\rangle\langle j|$. This is an idea that goes back to Dirac.(28) , where each quantum state is analogous to a harmonic oscillator. One can, if it proves useful, also consider such a Hamiltonian as being of an Ising type. This requires that one thinks of each 'spin' is a state and these states are pairwise coupled.

The evolution operator

Our aim is to determine explicitly the dynamical symmetries of the Hamiltonian and initial conditions as an explicit expression in terms of the time independent closed set of operators $\{\boldsymbol{A}_r\}$. To do so we need to propagate these operators in time. Actually, backwards in time. To move in time we need the evolution operators. For the given closed set of operators, and when the Hamiltonian is a linear expression of members of the set, equation (5), we follow the construction of Wei and Norman (8, 9) to obtain these. We caution already very early that while we use the approach of Wei and Norman to determine the evolution operator, the time correlation matrix that we are after is different from the time correlation matrix of Wei and Norman. Either matrix is tightly defined and there is a good reason why they are different. The matrix we require propagates the constraints backwards in time with the action of the full Hamiltonian of the system. It then expresses the dynamical symmetries as linear combinations, with time dependent coefficients, of the Schrödinger type operators.

The starting technical development is the parametrization of the time evolution operator in a product form as proposed by Wei and Norman (8, 9)

$$U(t) = \exp(g_1(t)X_1)\exp(g_2(t)X_2) \ldots \exp(g_\nu(t)X_\nu) \quad (7)$$

where ν is the number of generators of the algebra. From here on, we use the notation X_k to denote the generators that are skew-Hermitian operators, i.e. where the $\{-iX_k\}$ are Hermitian. With this condition the evolution operator $U(t)$ of equation (7) is unitary when the $\{g_k(t)\}$ are real.

The *N*-state system unitary evolution operator U is comprised of ν different factors $\exp(g_k X_k)$. The factors can be grouped into sets of three, each constituting an $SU(2)$ group. There are η groups with $\nu = 3\eta$. The three skew-Hermitian generators of each group are taken to involve two quantum states. Labelling the two quantum states i and *j,* the three generators of each $SU(2)$ subgroup have the form

$$X_a = i\left(E_{ij} + E_{ji}\right); X_b = \left(E_{ij} - E_{ji}\right); X_c = i\left(E_{ii} - E_{jj}\right) \quad (8)$$

where $E_{ij} = |i\rangle\langle j|$ is the coherence or, for $i = j$, the population observable. Sometimes the $\{E_{ij}\}$ are called Gelfand operators.

In the following we describe the factorization approach for one *SU*(2) group using the generators as shown in Equation (8). In the SI we construct the factorization of the evolution operator and the construction dynamical symmetries for the direct product of three *SU*(2) algebras, each one uses Equation (8). See also the work of Hioe and Eberly on three coupled states**(29)** .

Equation (8) is not the most common basis for $SU(2)$. It is a basis previously used to advantage by Altafini(7, 30) and in ref. (31) and it proves convenient for our purpose of computing the group parameters $\{g_k\}$ that, for the skew Hermitian operators X are then real for a unitary $\boldsymbol{U}$.

For a system of N quantum states there will be $\eta = N(N-1)/2$ distinct pairs of states so η is therefore the number of coupled $SU(2)$ systems. There are three generators X per each *SU*(2) so the total number of generators is $\nu = 3\eta$ The values of ν and η are given in Table 1 for different values of N.

Table 1: Lengths of unitary operators (ν) and numbers of directly coupled $SU(2)$ groups (η) for systems of N quantum states

N-State System	$\mathrm{U} = \prod_{i=1}^{\nu} \exp(g_i X_i)$	$\prod_1^{\eta} \otimes \mathrm{SU}(2)$

$N = 2$	$\nu = 3$	$\eta = 1$
$N = 3$	$\nu = 9$	$\eta = 3$
$N = 4$	$\nu = 18$	$\eta = 6$
N	$\nu = 3\eta$	$\eta = N(N-1)/2$

The dependence of the unitary operator on the set of parameters $\{g_k\}$ is

$$\partial U/\partial \mathrm{g}_k = \left(\prod_{j=1}^{k-1} \exp(g_j X_j)\right) X_k \left(\prod_{j=k}^{\nu} \exp(g_j X_j)\right) \quad (9)$$

To write this in a more compact form Wei and Norman define a matrix Ξ with, the elements ξ of which are defined as

$$(\partial U/\partial g_k)U^{-1} = \left(\prod_{j=1}^{k-1} \exp(g_j X_j)\right) X_k \left(\prod_{j=k-1}^{1} \exp(-g_j X_j)\right) \equiv \sum_{m=1}^{\nu} \xi_{mk} X_m \quad (10)$$

Here the matrix elements ξ_{mk} depend on $(\nu - 1)$ $g_k's$, $\xi_{mk}(g_1, g_2, \dots, g_{\nu-1})$. As defined, *m* is an index of a row of the Ξ matrix while *k* is an index of a column. See the SI Sections 1.1 and 2.1 for a full enumeration of the 2- and 3- state Ξ's respectively in the skew-Hermitian basis defined by equation (8). The matrix elements ξ_{mk}, through the $\{g_k(t)\}$, are functions of time, $\xi_{mk}\left(g_1(t), g_2(t), \dots, g_{\nu-1}(t)\right)$. As a function of the $\{g_k\}$, Ξ can therefore be determined from the commutation relations of the algebra without reference to any particular Hamiltonian. The correlation matrix $\Xi(g_1, g_2, \dots, g_{\nu-1})$ is an invertible, non-symmetric ν by ν matrix. Its specific form depends on the form of the operators used to close the algebra and of their order in Eq. (7). Using a notation of matrix algebra, an alternative form of the k^{th} column of the Ξ matrix is $\exp(g_1 adX_1)\exp(g_2 adX_2)\dots\exp(g_{k-1} adX_{k-1})X_k$ where the operation adX_m on an operator X_k is defined as $(adX_m)X_k = [X_m, X_k]$ so that $(adX_m)^2 X_k = \left[X_m, [X_m, X_k]\right]$ etc.

The equations of motion for the $\{g_k(t)\}$ are derived by differentiating (7) wrt to time, multiplying from the right by $U^{-1}(t)$, and then substituting into it the equation of motion of the evolution operator $i\,\partial U(t)/\partial t = H(t)U(t)$.

$$\partial U(t)/\partial t = \sum_k (\partial g_k/\partial\, t)\left(\prod_{j=1}^{k-1} \exp(g_j X_j)\right) X_k \left(\prod_{j=k}^{\nu} \exp(g_j X_j)\right)$$

$$(\partial U(t)/\partial t)U^{-1}(t) = \sum_k (\partial g_k/\partial\, t)\left(\prod_{j=1}^{k-1} \exp(g_j X_j)\right) X_k \left(\prod_{j=k-1}^{1} \exp(-g_j X_j)\right) \quad (11)$$

For the Hamiltonian that is linear in the generators (equation (5))

$$\sum_{k=1}^{\nu} h_k(t) X_k = i \sum_{k=1}^{\nu} (\partial g_k/\partial\, t)\left(\prod_{j=1}^{k-1} \exp(g_j X_j)\right) X_k \left(\prod_{j=k-1}^{1} \exp(-g_j X_j)\right)$$

$$\sum_{k=1}^{\nu} h_k(t) X_k = i \sum_{k=1}^{\nu} (\partial g_k/\partial\, t) \sum_{m=1}^{\nu} \xi_{mk}(g_1, g_2, \dots, g_\nu) X_m \quad (12)$$

(See the SI Section 1.1 for a more detailed derivation of equations (11) and (12)).

We wrote the matrix elements ξ_{mk} as functions of the $\{g_k\}$ because they are determined by the algebra for all the possibly time dependent Hamiltonians that are linear functions of the generators. The matrix Ξ is a real analytic function with an initial value of $\boldsymbol{I}$ at t =0. Since the generators are linearly independent we have explicit ν equations of motion separately for each one of the ν parameters of the evolution operator

$$dg_k/dt = \sum_k (\Xi^{-1})_{mk} h_k(t)\,,\ m = 1, \dots, \nu \tag{13}$$

We reiterate that the matrix Ξ is a function of the $\{g_k\}$. So the equations of motion are first order in time but they are not linear equations and they are coupled. The initial values for all are $g_k(t=0) = 0$ so that there is an explicit solution at least for very short times.

Dynamical symmetries for quantum computers

The first step is to extend the definition of the matrix elements, ξ_{mk}, equation (10), for all ν sets of parameters, $r = 1,2, \dots, \nu$

$$\left(\prod_{j=1}^{r} \exp(g_j X_j)\right) X_k \left(\prod_{j=r}^{1} \exp(-g_j X_j)\right) \equiv \sum_{m=1}^{\nu} \xi_{mk} X_m$$

$$\forall\, r = 1,2, \dots, \nu \quad \xi_{mk} = \xi_{mk}(g_1, g_2, \dots, g_r) \tag{14}$$

For the case r = ν , this expresses the full dynamical symmetry $X_k(t) = U(t) X_k U^\dagger(t)$ as a linear combination of time independent, Schrödinger picture, operators, equation (6)

$$X_k(t) = \sum_{j=1}^{\nu} a_{kj}(t) X_j \tag{15}$$

We next intend to demonstrate a computation of the dynamical symmetries in a manner particularly suitable for currently and near future quantum computers namely as coupled $SU(2)$ algebras, where each algebra is a coherent two-level system and so, a qubit. We will present analytical results for one qubit below and detailed analytical results for three coupled qubits in the supplementary information. Our tool, as already hinted earlier, is to write the Hamiltonian as a linear combination of the diagonal operators $|i\rangle\langle i|$ and the off diagonal ones $|i\rangle\langle j|$ where the $\{|i\rangle\}$ are the basis states, typically these are the eigenstates of the Hamiltonian in the absence of input so that, without input, the state of the system is stationary.

For the coupled qubits problem and to be consistent with the notation in Lie algebraic papers we use X_k's for the Schrödinger operators with $E_{ij} = |i\rangle\langle j|$. For a two-level system

$$\boldsymbol{I} = \boldsymbol{E}_{11} + \boldsymbol{E}_{22} \tag{16}$$

$$\boldsymbol{X}_1 = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix} = i(\boldsymbol{E}_{12} + \boldsymbol{E}_{21}) \tag{17}$$

$$\boldsymbol{X}_2 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = (\boldsymbol{E}_{12} - \boldsymbol{E}_{21}) \tag{18}$$

$$\boldsymbol{X}_3 = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} = i(\boldsymbol{E}_{11} - \boldsymbol{E}_{22}) \tag{19}$$

This is almost the same basis as was used by Altafini (7, 30) and in ref. (31) The input is provided by a time dependent pulse $E(t)$ so that the full Hamiltonian operator

$$H(t) = 0E_{11} - E(t)\mu E_{12} - E(t)\mu E_{21} + \alpha E_{22} \tag{20}$$

and in matrix form

$$\boldsymbol{H}(t) = \begin{pmatrix} 0 & -E(t)\mu \\ -E(t)\mu & \alpha \end{pmatrix} \tag{21}$$

The ground state is taken to be at energy zero so that α is the energy of excitation. Equation (21) can be rewritten in terms of the $SU(2)$ operators

$$\boldsymbol{H} = iE(t)\mu\boldsymbol{X}_1 + i\frac{\alpha}{2}\boldsymbol{X}_3 + \frac{\alpha}{2}\boldsymbol{I} \tag{22}$$

so that the vector of the coefficients of the operators in the Hamiltonian, $h(t)$ (see equation (5)) is

$$\boldsymbol{h}^T(t) = i(E(t)\mu \quad 0 \quad \alpha/2) \tag{23}$$

The commutation relations of the $SU(2)$ operators are given in Table 2.

Table 2: Commutation relations of the group $SU(2)$

	$[\cdot, X_1]$	$[\cdot, X_2]$	$[\cdot, X_3]$
$[X_1,\cdot]$	0	$-2X_3$	$2X_2$
$[X_2,\cdot]$	$2X_3$	0	$-2X_1$
$[X_3,\cdot]$	$-2X_2$	$2X_1$	0

The evolution operator is chosen to be in a sequential order of operators

$$U(t) = \exp(g_1(t)X_1)\exp(g_2(t)X_2)\exp(g_3(t)X_3) \tag{24}$$

where for our choice of skew-Hermitian operators $\{X_k\}$ we will need to verify that the results for the $\{g_k\}$ are real in order that the evolution operator is unitary.

Using the commutation table, Table 2, we compute the elements of the $\boldsymbol{\Xi}$ matrix that governs the time evolution of the $\{g_k\}$ (equation (13)), as follows. Looking first at column 1, which is $\exp(g_1 adX_1)X_1$. Because $\exp(g_1 adX_1)X_1 = X_1$, the first entry is $\xi_{11} = 1$ and the others are zero. Column 2 is $\exp(g_1 adX_1)X_2$, which can be expanded as a series

$$\exp(g_1 adX_1)X_2 = X_2 + g_1[X_1, X_2] + \frac{(g_1)^2}{2!}\big[X_1, [X_1, X_2]\big] + \frac{(g_1)^3}{3!}\Big[X_1, \big[X_1, [X_1, X_2]\big]\Big] \ldots \tag{25}$$

Inserting the commutator relation $[X_1, X_2] = -2X_3$ and then $[X_1, X_3] = 2X_2$ from Table 2, we get $\exp(g_1 adX_1)X_2 = (\cos(2g_1)\, X_2 - \sin(2g_1)\, X_3)$. Therefore, the only non-zero entries in column 2 are $\xi_{22} = \cos(2g_1)$ and $\xi_{32} = -\sin(2g_1)$.

To find column 3, $\exp(g_1 adX_1)\exp(g_2 adX_2)X_3$ requires two steps. First, we use a series expansion to show $\exp(g_2 adX_2)X_3 = (\cos(2g_2)\, X_3 - \sin(2g_2)\, X_1)$. We then multiply both sides of this equation on the left by $\exp(g_1 adX_1)$, and use the relations $\exp(g_1 adX_1)X_2 = (\cos(2g_1)\, X_2 - \sin(2g_1)\, X_3)$ and $\exp(g_1 adX_1)X_1 = X_1$ to acquire

$\exp(g_1 adX_1)\exp(g_2 adX_2)X_3 = -\sin(2g_2)\, X_1 + \cos(2g_2)\sin(2g_1)\, X_2 + \cos(2g_2)\cos(2g_1)\, X_3$

The elements of the third column are therefore $\xi_{13} = -\sin(2g_2)$, $\xi_{23} = \cos(2g_2)\sin(2g_1)$ and $\xi_{33} = \cos(2g_2)\cos(2g_1)$ (See SI Section 1.1 for a fully detailed derivation)

Using the entries in the three columns, the $\boldsymbol{\Xi}$ matrix and its inverse are

$$\boldsymbol{\Xi} = \begin{pmatrix} 1 & 0 & -\sin(2g_2) \\ 0 & \cos(2g_1) & \cos(2g_2)\sin(2g_1) \\ 0 & -\sin(2g_1) & \cos(2g_2)\cos(2g_1) \end{pmatrix}, \boldsymbol{\Xi}^{-1} = \begin{pmatrix} 1 & \tan(2g_2)\sin(2g_1) & \tan(2g_2)\cos(2g_1) \\ 0 & \cos(2g_1) & -\sin(2g_1) \\ 0 & \sec(2g_2)\sin(2g_1) & \sec(2g_2)\cos(2g_1) \end{pmatrix} \tag{26}$$

and from $\dot{\boldsymbol{g}} = -\mathrm{i}\boldsymbol{\Xi}^{-1}\boldsymbol{h}(\mathrm{t})$ (equation (13)) we get three coupled differential equations to find the $\{g_k(t)\}$

$$\begin{aligned} \dot{g_1} &= E(t)\mu + \frac{\alpha}{2}\tan(2g_2)\cos(2g_1) \\ \dot{g_2} &= -\frac{\alpha}{2}\sin(2g_1) \\ \dot{g_3} &= \frac{\alpha}{2}\sec(2g_2)\cos(2g_1) \end{aligned} \tag{27}$$

After solving these coupled differential equations for the $\{g_k(t)\}$ as a function of time we need an explicit form of the evolution operator, $U(t)$, either as a sum of the three generators or as a matrix. This form can then be applied to compute other observables or the initial density matrix vs. time.

To do so we expand the three exponentials that appear in the evolution operator as a power series. The first factor of equation (24) is

$$\exp(g_1 ad\boldsymbol{X}_1) = \boldsymbol{I} + g_1\boldsymbol{X_1} + \frac{(g_1\boldsymbol{X_1})^2}{2!} + \frac{(g_1\boldsymbol{X_1})^3}{3!} + \frac{(g_1\boldsymbol{X_1})^4}{4!} + \frac{(g_1\boldsymbol{X_1})^5}{5!} \ldots$$

Substituting in the relations that that $(\boldsymbol{X_1})^b = (i)^b(\boldsymbol{E}_{12} + \boldsymbol{E}_{21})\ \forall\, b$ odd, and $(\boldsymbol{X_1})^b = (i)^b(\boldsymbol{E}_{11} + \boldsymbol{E}_{22})\ \forall\, b$ even, the two practical forms for the first exponential in the evolution operator are obtained

$$\exp(g_1 ad\boldsymbol{X}_1) = \begin{pmatrix} \cos(g_1) & i\sin(g_1) \\ i\sin(g_1) & \cos(g_1) \end{pmatrix} \quad (28)$$

and

$$\exp(g_1 ad\boldsymbol{X}_1) = \left(\cos(g_1)\boldsymbol{I} + i\sin(g_1)(\boldsymbol{E}_{12} + \boldsymbol{E}_{21})\right) \quad (29)$$

Expanding out $\exp(g_2 ad\boldsymbol{X}_2)$ as a power series, and substituting $(\boldsymbol{X_2})^b = (i)^{b-1}(\boldsymbol{E}_{12} - \boldsymbol{E}_{21})\ \forall\, b$ odd, and $(\boldsymbol{X_2})^b = (i)^b(\boldsymbol{E}_{11} + \boldsymbol{E}_{22})\ \forall\, b$ even, yields

$$\exp(g_2 ad\boldsymbol{X}_2) = \left(\cos(g_2)\boldsymbol{I} + \sin(g_2)(\boldsymbol{E}_{12} - \boldsymbol{E}_{21})\right) = \begin{pmatrix} \cos(g_2) & \sin(g_2) \\ -\sin(g_2) & \cos(g_2) \end{pmatrix} \quad (30)$$

Finally for the third exponential, substituting $(\boldsymbol{X_3})^b = (i)^b(\boldsymbol{E}_{11} - \boldsymbol{E}_{22})\ \forall\, b$ odd, and $(\boldsymbol{X_3})^b = (i)^b(\boldsymbol{E}_{11} + \boldsymbol{E}_{22})\ \forall\, b$ even into the $\exp(g_3 ad\boldsymbol{X}_3)$ power series yields

$$\exp(g_3 ad\boldsymbol{X}_3) = \left(e^{ig_3}\boldsymbol{E}_{11} + e^{-ig_3}\boldsymbol{E}_{22}\right) = \begin{pmatrix} e^{ig_3} & 0 \\ 0 & e^{-ig_3} \end{pmatrix} \quad (31)$$

Multiplying the three matrices we get a matrix representation for the evolution operator of a two state system

$$\boldsymbol{U} = \begin{pmatrix} e^{ig_3}\left(\cos(g_1)\cos(g_2) - i\sin(g_1)\sin(g_2)\right) & e^{-ig_3}\left(\cos(g_1)\sin(g_2) + i\sin(g_1)\cos(g_2)\right) \\ -e^{ig_3}\left(\cos(g_1)\sin(g_2) - i\sin(g_1)\cos(g_2)\right) & e^{-ig_3}\left(\cos(g_1)\cos(g_2) + i\sin(g_1)\sin(g_2)\right) \end{pmatrix} \quad (32)$$

To compute the dynamical symmetries, and because $\boldsymbol{U}$ is unitary, we also need its inverse

$$\boldsymbol{U^{-1}} = \begin{pmatrix} e^{-ig_3}\left(\cos(g_1)\cos(g_2) + i\sin(g_1)\sin(g_2)\right) & -e^{-ig_3}\left(\cos(g_1)\sin(g_2) + i\sin(g_1)\cos(g_2)\right) \\ e^{ig_3}\left(\cos(g_1)\sin(g_2) - i\sin(g_1)\cos(g_2)\right) & e^{ig_3}\left(cos(g_1)\,cos(g_2) - i\sin(g_1)\sin(g_2)\right) \end{pmatrix} \quad (33)$$

The form of the dynamical symmetry operators is $\mathcal{X}_k = UX_kU^{-1}$. The three dynamical symmetries in operator sum form are

$$\mathcal{X}_1 = \cos(2g_2)\cos(2g_3)\,X_1 + \left(\sin(2g_1)\sin(2g_2)\cos(2g_3) - \cos(2g_1)\sin(2g_3)\right)X_2 + \left(\cos(2g_1)\sin(2g_2)\cos(2g_3) + s\text{in}(2g_1)\sin(2g_3)\right)X_3$$

$$\mathcal{X}_2 = \cos(2g_2)\sin(2g_3)\,X_1 + \left(\cos(2g_1)\cos(2g_3) + \sin(2g_1)\sin(2g_2)\sin(2g_3)\right)X_2 + \left(\cos(2g_1)\sin(2g_2)\sin(2g_3) - \sin(2g_1)\cos(2g_3)\right)X_3$$

$$\mathcal{X}_3 = -\sin(2g_2)\,X_1 + \sin(2g_1)\cos(2g_2)\,X_2 + \cos(2g_1)\cos(2g_2)\,X_3 \quad (34)$$

The time correlation matrix from the Schrödinger picture to the dynamical symmetries, equation (14), is thereby given as

$$\boldsymbol{\Xi}_{\boldsymbol{dynsym}} = \begin{pmatrix} \xi_{11}^{DS} & \xi_{12}^{DS} & \xi_{13}^{DS} \\ \xi_{21}^{DS} & \xi_{22}^{DS} & \xi_{23}^{DS} \\ \xi_{31}^{DS} & \xi_{32}^{DS} & \xi_{33}^{DS} \end{pmatrix}$$

where

$\xi_{11}^{DS} = \cos(2g_2)\cos(2g_3)$

$\xi_{12}^{DS} = \sin(2g_1)\sin(2g_2)\cos(2g_3) - \cos(2g_1)\sin(2g_3)$

$\xi_{13}^{DS} = \cos(2g_1)\sin(2g_2)\cos(2g_3) + \sin(2g_1)\sin(2g_3)$

$\xi_{21}^{DS} = \cos(2g_2)\sin(2g_3)$

$\xi_{22}^{DS} = \sin(2g_1)\sin(2g_2)\sin(2g_3) + \cos(2g_1)\cos(2g_3)$

$\xi_{23}^{DS} = \cos(2g_1)\sin(2g_2)\sin(2g_3) - \sin(2g_1)\cos(2g_3)$

$\xi_{31}^{DS} = -\sin(2g_2)$

$\xi_{32}^{DS} = \sin(2g_1)\cos(2g_2)$

$\xi_{33}^{DS} = \cos(2g_1)\cos(2g_2)$ (35)

The time correlation matrix from the Schrödinger picture to the Heisenberg operators is

$$\Xi_H = \begin{pmatrix} \xi_{11}^{H} & \xi_{12}^{H} & \xi_{13}^{H} \\ \xi_{21}^{H} & \xi_{22}^{H} & \xi_{23}^{H} \\ \xi_{31}^{H} & \xi_{32}^{H} & \xi_{33}^{H} \end{pmatrix}$$

where

$\xi_{11}^{H} = \cos(2g_2)\cos(2g_3)$

$\xi_{12}^{H} = \cos(2g_2)\sin(2g_3)$

$\xi_{13}^{H} = -\sin(2g_2)$

$\xi_{21}^{H} = \sin(2g_1)\sin(2g_2)\cos(2g_3) - \cos(2g_1)\sin(2g_3)$

$\xi_{22}^{H} = \sin(2g_1)\sin(2g_2)\sin(2g_3) + \cos(2g_1)\cos(2g_3)$

$\xi_{23}^{H} = \sin(2g_1)\cos(2g_2)$

$\xi_{31}^{H} = \cos(2g_1)\sin(2g_2)\cos(2g_3) + \sin(2g_1)\sin(2g_3)$

$\xi_{32}^{H} = \cos(2g_1)\sin(2g_2)\sin(2g_3) - \sin(2g_1)\cos(2g_3)$

$\xi_{33}^{H} = \cos(2g_1)\cos(2g_2)$ (36)

The dynamical symmetries are Heisenberg operators that move backwards in time, and one verifies that the two time correlation matrices are indeed inverse to one another. For more detailed results of the two-state system see section 1 of the SI.

Using the evolution operator one can propagate in time any initial state that can be specified by the three generators, $\rho(t) = U(t)\rho(t=0)U^{-1}(t)$. When at time zero the system is in its ground state

$$\boldsymbol{\rho}(\mathrm{t}) = \boldsymbol{U}(t)\begin{pmatrix}1 & 0\\0 & 0\end{pmatrix}\boldsymbol{U}^{-1}(t) = \exp\left(\boldsymbol{U}(t)\left(\tfrac{1}{2}(\boldsymbol{I} - i\boldsymbol{X}_3)\right)\boldsymbol{U}^{-\mathbf{1}}(t)\right) = \exp\left(\tfrac{1}{2}(\boldsymbol{I} - i\boldsymbol{\mathcal{X}}_{\mathbf{3}}(t))\right) =$$

$$\begin{pmatrix}\rho_{11} & \rho_{12}\\ \rho_{21} & \rho_{22}\end{pmatrix}$$

where

$$\rho_{11} = \cos^2(g_1)\cos^2(g_2) + \sin^2(g_1)\sin^2(g_2)$$
$$\rho_{12} = -\big(\cos(g_1)\sin(g_2) + i\sin(g_1)\cos(g_2)\big)(\cos(g_1)\cos(g_2) - i\sin(g_1)\sin(g_2))$$
$$\rho_{21} = i\left(\sin(g_1)\cos(g_2) + i\cos(g_1)\sin(g_2)\right)(\cos(g_1)\cos(g_2) + i\sin(g_1)\sin(g_2))$$
$$\rho_{22} = \sin^2(g_1)\cos^2(g_2) + \cos^2(g_1)\sin^2(g_2) \qquad (37)$$

The final matrix form is an explicit result and shows that the elements of the density matrix of Maximal Entropy are not necessarily simple exponentials.

Matrix multiplication explicitly verifies that the expectation values of the dynamical symmetries for the density matrix at time *t* are time independent and equal to the initial values of the generators (that are 0, 0 and i respectively – see SI section 1.3.3, equations (S37), (S38) and (S39) for full details).

Concluding Remarks

A practical approach to computing quantum dynamical symmetries is discussed and implemented. In the supplementary information, SI, file we apply it to a system of three coupled two state systems (= qubits) $SU(2) \otimes SU(2) \otimes SU(2)$ which shows the connection to quantum computing designs and to Ising Hamiltonians. For optical addressing the Hamiltonian can be written as ($H = \sum_{i,j} H_{ij}\, |i\rangle\langle j|$) and it is of an Ising form when each quantum level is encoded on the spin state of a qubit. One can choose the three generators for each *SU*(2) algebra such that the factorized evolution operator is guaranteed unitary. The factorization is two fold. Each *SU*(2) algebra results in its own factor in the evolution operator and each such factor is a sequence of terms, one for each of the three generators, see Table 1. As reported in detail in the SI, this leads to a very stable numerical scheme even for strong coupling. Using the dynamical symmetries we construct quantum mechanical distributions of maximal entropy. Explicit results for systems with coherences show that populations are not necessarily simple exponentials and are often a sum of terms. It may be of interest to draw an analogy with classical distributions of maximal entropy. These can also be not a single exponential for example when there are several paths leading to the same final state. If $P(j,n)$ is the probability of state *j* via the distinct path *n* and $P(j)$ is the total probability of the state, then $P(j) = \sum_n P(j,n)$. It remains to be clearly understood if this is analogous to the inherently parallel processing in quantum dynamics. One can suggest that while in Boolean logic events do or do not happen, probable inference(32, 33) is a generalization of logic to events that have a finite probability of occurring. In this paper we implemented an algebraic approach for the explicit computation of quantum probabilities in particular for systems that evolve in time and when the Hamiltonian can be written as a matrix. Then the states of the system are pairwise coupled and the dynamics can be cast as coupled two state systems.

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Supplementary information: The SI provides the details of the derivations of the results of the coupled 2 state SU(2) system discussed in the main text and the derivation for the three coupled 2 state problem cast as SU(2)⨂SU(2)⨂SU(2).

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