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Exact mapping of the quantum states in arbitrary N-level systems to the positions of classical coupled oscillators

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The quantum dynamics of arbitrary N-level systems, including dissipative systems, are modeled exactly here by the dynamics of classical coupled oscillators. A one-to-one correspondence is established between the quantum states and the positions of the oscillators. Quantum coherence, expectation values, and measurement probabilities for system observables can therefore be realized from the corresponding classical states. Although the well-known equivalence ($SU(2)$, $SO(3)$ homomorphism) of 2-level quantum dynamics to a rotation in real, physical space cannot be generalized to arbitrary N-level systems, the representation of quantum dynamics by a system of coupled harmonic oscillators in one physical dimension *is* general for any N. The time evolution of an N-level system (generated by a complex element of the $SU(N)$ group), is first represented as the rotation of a real state vector in (unphysical) hyperspace, as previously known for density matrix states and also extended here to include Schrödinger states. The resulting rotor in n Euclidean dimensions (the rotation group $SO(n)$) is then mapped directly to n oscillators in one physical dimension, which significantly reduces the level of abstraction required to visualize quantum dynamics compared to vector models or generalized Bloch spheres in higher dimensions. The number of such oscillators needed to represent N-level systems scales as N^2 for the density matrix formalism but increases only linearly with N for Schrödinger states. Values for the classical coupling constants are readily derived from the system Hamiltonian, allowing construction of classical mechanical systems that provide insight into the dynamics of abstract quantum systems (new dynamical invariants) as well as a metric for characterizing the interface between quantum and classical mechanics. A distinctive attribute of the quantum-classical connection as presented here is the necessity for both positive and negative couplings, and, in the case of dissipative systems, antisymmetric couplings.

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I. INTRODUCTION.

The density matrix formalism [1–3] provides a straightforward procedure for predicting quantum dynamics, applicable very generally to pure states, statistical mixtures of pure states, and dissipative (open) systems. Although the theory needs no supporting visual model for its application, the Liouville-von Neumann equation governing the time evolution of the density matrix provides little physical insight into system dynamics. There has therefore been considerable effort towards representing, where possible, quantum systems using more intuitive classical models. Of particular influence and importance is the classical representation for quantum two-level systems [4], sometimes referred to as the Feynman–Vernon–Hellwarth (FVH) Theorem. The behavior of any quantum mechanical two-level system can be modeled by classical torque equations, providing a one-to-one correspondence between the time evolution of the system and the dynamics of, for example, a spinning top in a constant gravitational field or a magnetic moment in a constant magnetic field.

Work by Fano [3] published concurrently with the FVH result also provides geometrical interpretation of spin dynamics for more complex quantum systems. The density

matrix for an N-level system is represented as an expansion in Hermitian operators, resulting in a vector with real components. The time development of this generalized Bloch vector is a real rotation in a hyperspace of $(N^2 - 1)$ dimensions. Constants of the motion can be derived [5, 6] that constrain the system’s dynamics and provide physical insight. However, the states of the system as given by the components of this vector (also referred to as a coherence vector [5] and, more recently, a Stoke’s tensor [7]), do not evolve in a physical space amenable to visualization, with its attendant advantages, except for the case $N = 2$.

Thus, no completely general mapping has been realized that yields a one-to-one correspondence between the states of a quantum-mechanical N-level system and classical dynamical variables. Interest in this topic is motivated by the success of the FVH result in providing direct physical insight into the dynamics of abstract quantum systems. For example, as observed in [8], the language and concepts of quantum optics have been heavily influenced by the FVH result.

Analogies between quantum and classical systems have been noted [9–21] almost from the beginning. But an equivalence between the quantum and classical equations of motion has been obtained only for certain limiting conditions [22–29] such as weak perturbations of the system (weak coupling limit) and the aforementioned 2-level systems.

Recently, the possibility of representing a subset of N-

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level quantum systems exactly in terms of classical coupled oscillators was demonstrated [30], with no restriction to weak coupling. However, this approach is limited at the outset to real Hamiltonians, and can only be applied to pure states evolving according to the time-dependent Schrödinger equation. Moreover, the quantum states must be inferred, somewhat indirectly, from the position, the velocity, and, subsequently, the conjugate momentum of each oscillator. The momentum is calculated as the inverse of the Hamiltonian times the velocity, which imposes a further restriction—invertibility—to the subset of relevant Hamiltonians. In a broader context, this approach is insufficiently general to establish a similar classical representation for statistical mixtures and density matrix evolution, which also precludes open, dissipative systems and important applications to decoherence.

In the present work, a very general, exact method is introduced for mapping arbitrary N -level quantum systems directly to the positions of coupled harmonic oscillators, undertaken by the author many years ago. It solves a problem of longstanding interest and is made more relevant now by recently published results [21, 30] on the quantum-classical connection. Given the ubiquity of the harmonic oscillator in modeling a host of important physical phenomena, this work should have significant implications beyond the basic formalism and examples of its implementation presented here.

The outline of the paper is as follows. The salient features for representing the dynamics of N -level systems as real rotations derived from the Liouville-von Neumann equation, rather than the usual complex rotations generated by $SU(N)$ group operators, are reviewed first. There is no restriction to real Hamiltonians and, most importantly, the formalism is applicable to both pure and mixed states. The desired one-to-one correspondence between the states of the quantum system, represented as a density matrix, and classical dynamical variables in real, physical space is provided by a mapping to harmonic oscillators. In contrast to the results in [30], the quantum states, either pure or mixed, are represented exactly using only the time-dependent displacements of classical coupled oscillators rather than the displacement, velocity, and conjugate momentum originally required. The Hamiltonian does not have to be invertible because it does not need to be inverted. The recipe for determining the physical couplings to construct the oscillator system completes the basic formalism, which will also be shown to be applicable to dissipative systems.

Although the treatment in terms of the density matrix provides a complete and general formalism for the quantum-classical mapping, the Schrödinger approach to this problem also warrants further consideration. Removing limitations of this approach might provide additional useful options and insights for characterizing the quantum-classical connection. Hilbert space rotations are therefore reviewed to generalize this option for representing the quantum dynamics of pure states classically.

Restrictions in the Schrödinger approach to real, invertible Hamiltonians are removed by recasting the time-dependent Schrödinger equation as a real equation. Its solution is then a rotation in real space as opposed to the usual rotation in a complex Hilbert space. (This is not the same as quantum mechanics in a real Hilbert space [31], although the points of departure are similar.) An exact one-to-one mapping of Schrödinger states to the physical displacements of coupled oscillators then follows immediately from the formalism developed thus far. Whereas $n = N^2 - 1$ classical oscillators are needed most generally to represent density matrix dynamics for an N -level system, Schrödinger states require at most $n = 2N$ oscillators, which can be reduced to N if the Hamiltonian is real. The present work therefore establishes an equivalence among complex $SU(N)$ rotations, real rotations in n Euclidean dimensions (i.e., the $SO(n)$ group), and systems of n coupled harmonic oscillators in one dimension, which may be relevant for other representations of quantum dynamics, such as the generalized Bloch sphere [32, 33]. Both positive and negative couplings are required most generally, which is a distinctive feature of the quantum-classical connection as presented here.

For the sake of completeness, the Schrödinger approach for representing spin dynamics is then extended to mixed states, although this most generally requires $2N^2$ oscillators and would not typically be preferred to the Liouville approach. However, as noted later, each Schrödinger pure state comprising the density matrix evolves independently of the others. Its precise contribution to system dynamics is readily discerned, providing an option for further insight.

Open (dissipative) N -level systems are considered next, showing they also can be exactly modeled as classical coupled oscillators. Dissipation is generated in ideal, frictionless oscillators by antisymmetric couplings. Such couplings emerge naturally as a result of extending the formalism presented so far to open systems. In this case, the Liouville approach developed here for the quantum-classical mapping is essential for applications that are not restricted to population relaxation or the simplest mechanisms for dephasing—for example, more general treatments of decoherence and cross-relaxation.

Illustrative examples of the quantum-classical mapping are then provided. The examples demonstrate the necessity for negative couplings in closed systems as well as antisymmetric couplings in open systems. The paper closes with the introduction of new invariants (constants of the motion) that may be useful in characterizing system dynamics and symmetries. The transition from the exact results to approximations that assume weak couplings at the outset of the analysis is provided in an Appendix.

II. TIME EVOLUTION OF

CLOSED N-LEVEL SYSTEMS

A brief synopsis of the standard Liouville and Hilbert space formalisms for representing the unitary time evolution of (closed) N-level systems serves as the contextual background for the quantum-classical connection established here. The time evolution of the system in both representations is first reduced to a rotation in real Euclidean space of the form

$$\Phi(t) = U(t) \Phi(0). \quad (1)$$

The chosen representation determines the particular form for the quantum state Φ and the propagator (unitary rotation operator) $U(t)$. A straightforward mapping of real rotations to classical coupled oscillators then follows. The Liouville formalism is considered first, since it provides the most general framework for the quantum-classical connection. It is readily extended in a subsequent section to dissipative systems that cannot be represented using the Schrödinger equation. For notational convenience and interchangeability of energy and frequency units, \hbar is set equal to 1 in what follows.

A. Liouville equation

The Liouville-von Neumann equation for the time evolution of a density matrix ρ governed by system Hamiltonian H is

$$\dot{\rho} = -i[H, \rho], \quad (2)$$

with formal solution

$$\begin{aligned} \rho(t) &= e^{-iHt} \rho(0) e^{iHt} \\ &= U \rho(0) U^\dagger, \end{aligned} \quad (3)$$

which defines $U(t) = e^{-iHt}$.

The time evolution can be related to a rotation by first expanding ρ in terms of a complete set of basis operators [3]. Orthogonal bases are particularly convenient and are typically normalized for further convenience. Denoting the basis elements as \hat{e}_i for state i and requiring only that the basis be orthonormal gives

$$\langle \hat{e}_i | \hat{e}_j \rangle = \text{Tr}(\hat{e}_i^\dagger \hat{e}_j) = \delta_{ij}, \quad (4)$$

where the inner product for the vector space comprised of matrices is given by the operator Tr , which returns the trace (sum of diagonal elements) of its argument. The symbol \dagger denotes the operation of Hermitian conjugation. In lieu of explicitly normalizing the \hat{e}_i , the inner product can be defined with the appropriate factor multiplying Tr . Then, ρ can be represented as

$$\rho = \sum_j r_j \hat{e}_j \quad (5)$$

where the coefficients in the expansion are the projection onto the basis states. Each r_j in Eq. (5),

$$r_j = \langle \hat{e}_j | \rho \rangle = \text{Tr}(\hat{e}_j^\dagger \rho), \quad (6)$$

is thus the expectation value of the quantum state \hat{e}_j .

Then

$$\begin{aligned} \dot{r}_i &= \text{Tr}(\hat{e}_i^\dagger \dot{\rho}) = -i \text{Tr}(\hat{e}_i^\dagger [H, \rho]) \\ &= \sum_j -i \text{Tr}(\hat{e}_i^\dagger [H, \hat{e}_j]) r_j \\ &= \sum_j \Omega_{ij} r_j. \end{aligned} \quad (7)$$

Expanding the commutator, using $\text{Tr}(AB) = \text{Tr}(BA) = [\text{Tr}(AB)^\dagger]^*$ and $[\hat{e}_i^\dagger, \hat{e}_j]^\dagger = [\hat{e}_j^\dagger, \hat{e}_i]$ gives

$$\begin{aligned} \Omega_{ij} &= -i \text{Tr}(\hat{e}_i^\dagger [H, \hat{e}_j]) \\ &= i \text{Tr}([\hat{e}_i^\dagger, \hat{e}_j] H) \\ &= -\{i \text{Tr}([\hat{e}_j^\dagger, \hat{e}_i] H)\}^* \\ &= -\Omega_{ji}^* \end{aligned} \quad (8)$$

in terms of its complex conjugate elements, denoted by * . Thus, $\Omega = -\Omega^\dagger$ is antihermitian and can be diagonalized. The evolution of the density matrix is given by

$$\dot{\mathbf{r}} = \Omega \mathbf{r}, \quad (9)$$

with solution

$$\mathbf{r}(t) = e^{\Omega t} \mathbf{r}(0). \quad (10)$$

The propagator $U(t) = e^{-iHt}$, and therefore $U^\dagger = U^{-1}$ is unitary, since $\Omega^\dagger = -\Omega$. Thus, Eq. (9) represents a rotation, albeit still most generally in complex space.

1. Rotation in real space

An orthonormal basis of Hermitian operators can always be found for N-level systems (for example, the generators of $\text{SU}(N)$). Choosing Hermitian basis states ensures that the components of the density matrix are real, and Ω derived from Eq. (8) is also a real antisymmetric matrix. The rotation of Eq. (9) is then a rotation in real, multidimensional space, which is the generalization of the FVH result [4] to N-level systems [3, 5]. More formally, the generator of the rotation, Ω , can be represented as a linear combination of the generators for $\text{SO}(n)$, the group of rotations about a fixed point in n -dimensional Euclidean space. Omitting the identity element in Eq. (5), which commutes with everything and produces a time-independent component in Eq. (7), gives $n = N^2 - 1$ starting with the N^2 elements of ρ .

The quantum dynamics are thus fully classical in the additional dimensions exceeding 3D physical space. However, classical rotations in more than three dimensions

are only marginally less abstract than rotations in a complex Hilbert space. More accessible insight can be obtained by mapping the transformed, real-valued quantum states to physical space. The mapping proceeds from complex $SU(N)$ to $SO(n)$ —describing a rotor in n real, Euclidean dimensions—to n classical oscillators in one physical dimension. The relation between $SU(N)$ and $SO(n)$ has applications to the generalized Bloch sphere [32, 33]. The broader relevance of mapping $SO(n)$ to one-dimensional oscillators warrants further investigation which is beyond the scope of the present article.

2. Exact mapping to classical coupled oscillators

A textbook exercise for deriving the Larmor precession of a spin-1/2 in a static magnetic field B_0 differentiates the first-order derivative in Ehrenfest's theorem. The result is a harmonic oscillator equation for the expectation values of the spin components transverse to B_0 . Similarly, differentiating Eq. (9) gives

$$\ddot{\mathbf{r}} = \Omega^2 \mathbf{r}. \quad (11)$$

Since Ω^2 is real, symmetric, and therefore diagonalizable, the solution is readily written in terms of the usual normal-mode solutions. Moreover, the eigenvalues, $-\omega_a^2$ ($a = 1, 2, 3, \dots, n$), for $n \times n$ matrix Ω^2 are guaranteed to be negative, since the eigenvalues of antihermitian Ω are pure imaginary. The n distinct eigenvectors $|\omega_a\rangle$ constitute a basis set satisfying the completeness relation $\sum_a |\omega_a\rangle\langle\omega_a| = \mathbb{1}$ (the identity element). In this eigenbasis, Eq. (11) for each component $r_a = \langle\omega_a|\mathbf{r}\rangle$ is, of course,

$$\ddot{r}_a = -\omega_a^2 r_a \quad (12)$$

with standard harmonic oscillator solution

$$r_a(t) = r_a(0) \cos \omega_a t + \frac{\dot{r}_a(0)}{\omega_a} \sin \omega_a t \quad (13)$$

and $\dot{\mathbf{r}}$ dependent on \mathbf{r} according to Eq. (9), giving

$$\begin{aligned} |r(t)\rangle &= \sum_{a=1}^n |\omega_a\rangle\langle\omega_a|r(t)\rangle \\ &= \sum_{a=1}^n |\omega_a\rangle\langle\omega_a| \left[\cos \omega_a t + \Omega \frac{\sin \omega_a t}{\omega_a} \right] |r(0)\rangle \\ &= U(t) |r(0)\rangle. \end{aligned} \quad (14)$$

Using the original representation for non-diagonal Ω^2 and its eigenvectors to calculate $U(t)$ gives the physical displacements $r_i(t)$ for each of the n oscillators. This solution for $U(t)$ must be identical to the propagator given in Eq. (10). It is included primarily for consistency in the presentation, but also to emphasize the fundamental differential equation under consideration is first order and only requires specification of $\mathbf{r}(0)$.

3. Classical coupling constants

To complete the explicit identification of Eq. (11) with mechanical oscillators, consider equal (unit) masses, m , on a frictionless surface, with mass m_i connected by spring of stiffness $k_{ij} = k_{ji}$ to mass m_j ($i, j = 1, 2, 3, \dots, n$), as in Fig. 1 for an illustrative case $n = 3$. The classical matrix Ω_{Cl} relating the displacement from

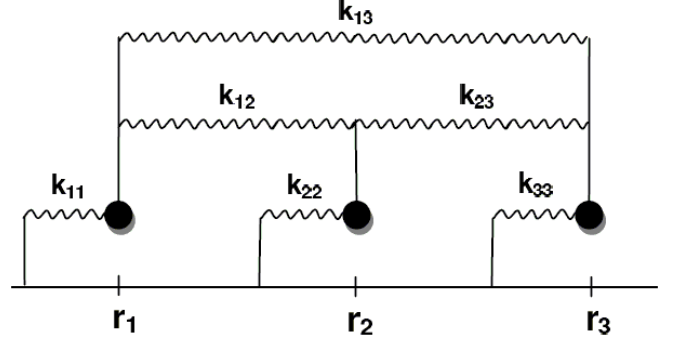


FIG. 1. Schematic of three masses at equilibrium positions $r_i = 0$ coupled with springs of stiffness k_{ij} .

equilibrium of the i^{th} mass to its acceleration, as in Eq. (11), is

$$(\Omega_{\text{Cl}})_{ij} = \frac{1}{m} \begin{cases} k_{ij} & i \neq j \\ -\sum_{l=1}^n k_{il} & i = j \end{cases} \quad (15)$$

for positive couplings k_{ij} .

However, negative couplings also arise quite naturally in the results which follow. A system of pendulums consisting of masses attached to rigid rods can be coupled negatively by attaching a spring to rod i below the fulcrum of oscillation and to rod j above the fulcrum. Displacing mass m_i to the right exerts a force on m_j to the left, ie, the coupling $k_{ij} < 0$. Yet, the force on m_i is still a restoring force, so $|k_{il}|$ must be used for the diagonal elements $i = j$ in Eq. (15) to accommodate negative couplings. A pendulum can be inverted with its mass above the fulcrum to implement $k_{ii} < 0$. Inverting transformers can be used to implement negative couplings in LC circuits.

Setting $\Omega_{\text{Cl}} = \Omega^2$ and using $|k_{il}| = |(\Omega^2)_{il}|$ to calculate the self-couplings k_{ii} gives the spring constants

$$\frac{k_{ij}}{m} = \begin{cases} (\Omega^2)_{ij} & i \neq j \\ -[(\Omega^2)_{ii} + \sum_{l \neq i} |(\Omega^2)_{il}|] & i = j \end{cases} \quad (16)$$

in terms of the matrix Ω (squared) representing the quantum system, as derived from Eq. (8). There is thus a one-to-one mapping of the quantum states to the oscillator displacements embodied in $r_i(t)$ for both systems. Given the initial states $r_i(0)$ of the system, the necessary $\dot{r}_i(0)$ follow from Eq. (9).

This mapping is very general. It is not limited to particular values of the spin, numbers of interacting spins, specific forms of the commutation relations, or relative fractions of mixed and pure states comprising ρ . An $N \times N$ density matrix generates N^2 components in Eq. (5), which requires N^2 oscillators. The static component of the identity element can be eliminated, and the structure of the Hamiltonian may generate evolution restricted to a smaller subspace of states, further reducing the number of required oscillators.

For pure states, the time-dependent elements $c_i(t)$ comprising the state vector can readily be obtained, if desired, from ρ reconstructed in matrix form using the $r_i(t)$ and Eq. (5). Each resulting element ρ_{ij} is equal to $c_i c_j^*$. Assigning any one of the c_i to the square root of ρ_{ii} sets the arbitrary global phase of the pure-state elements. In terms of this real c_i , the remaining c_j are equal to ρ_{ji}/c_i .

As will be shown next, a mapping, for complex H , of pure states in the Schrödinger picture to at most $2N$ oscillators is also possible. However, dissipative systems, which cannot most generally be described by pure states, still require on the order of N^2 .

B. Schrödinger equation

The solution

$$|\Psi(t)\rangle = e^{-iHt} |\Psi(0)\rangle. \quad (17)$$

to the time-dependent Schrödinger equation

$$i|\dot{\Psi}(t)\rangle = H|\Psi(t)\rangle \quad (18)$$

represents a rotation of $|\Psi(0)\rangle$ in Hilbert space, since H is Hermitian and the propagator $U(t) = e^{-iHt}$ is unitary. Most generally, H and the components c_i of $|\Psi\rangle$ in a chosen basis are complex, so a classical interpretation for the time evolution of the state is not readily apparent.

In [30], the authors present an approach for representing the complex c_i in terms of the displacements and conjugate momenta of classical coupled oscillators, restricted to the special case of real, invertible H . These restrictions can be removed, as will be shown in what follows. The formalism of the previous sections can be applied to the Schrödinger equation by recasting it in the form of a real rotation for general H .

1. Rotation in real space

Many previous investigations of quantum-classical connections [9, 10, 21, 30] focus on the Hamilton equations of motion. They start with a real, classical Hamiltonian \mathcal{H} and relate it to the quantum Hamiltonian, H . The outcome in [30] is that \mathcal{H} represents real harmonic oscillators only if the quantum H is real, which is then applied to the Schrödinger equation.

The formalism of the preceding sections, which accommodates general, complex H , can be extended directly to the Schrödinger equation without reference to the Hamilton equations. Start with Eq. (18) and represent the components of $|\Psi\rangle$ for an N -level system as an N -component vector \mathbf{c} in the usual manner, giving

$$\dot{\mathbf{c}}(t) = -iH\mathbf{c}(t). \quad (19)$$

Write complex $\mathbf{c} = \mathbf{q} + i\mathbf{p}$ and complex $H = Q + iP$. Equating the real and imaginary parts after performing the multiplications in Eq. (19) recasts the Schrödinger equation as a real equation

$$\begin{pmatrix} \dot{\mathbf{q}} \\ \dot{\mathbf{p}} \end{pmatrix} = \begin{pmatrix} P & Q \\ -Q & P \end{pmatrix} \begin{pmatrix} \mathbf{q} \\ \mathbf{p} \end{pmatrix} = \Omega \begin{pmatrix} \mathbf{q} \\ \mathbf{p} \end{pmatrix} \quad (20)$$

in the form of Eq. (9) with $\Omega^\dagger = -\Omega$ real, antisymmetric, since Hermitian H requires $Q^\dagger = Q$ and $P^\dagger = -P$. The results and implications for real rotations then follow from §II A 1 and the discussion following Eq. (9). There are $2N$ real parameters $(q_1, \dots, q_N, p_1, \dots, p_N)$ comprising the N complex elements of $|\Psi\rangle$. Schrödinger equation evolution of N -level systems can therefore be represented as rotations in real $2N$ -dimensional Euclidean space. In principle, this can be reduced to $2(N-1)$ by the normalization condition and choice of a specific value (typically zero) for the arbitrary and physically meaningless global phase of the state vector [3].

A search of the literature uncovers research developing quantum mechanics in a real Hilbert space [31] that configures the state vector as $(q_1, p_1, \dots, q_N, p_N)$. The associated Hamiltonian is then neither symmetric or antisymmetric. The analogue to Eq. (20) is not a real rotation, so this particular representation misses the possibility of mapping a real time-dependent Schrödinger equation to classical coupled oscillators.

2. Exact mapping to classical coupled oscillators

Differentiating Eq. (20) gives

$$\begin{aligned} \begin{pmatrix} \ddot{\mathbf{q}} \\ \ddot{\mathbf{p}} \end{pmatrix} &= \begin{pmatrix} P & Q \\ -Q & P \end{pmatrix}^2 \begin{pmatrix} \mathbf{q} \\ \mathbf{p} \end{pmatrix} \\ &= \begin{pmatrix} P^2 - Q^2 & PQ + QP \\ -(PQ + QP) & P^2 - Q^2 \end{pmatrix} \begin{pmatrix} \mathbf{q} \\ \mathbf{p} \end{pmatrix} \\ &= \begin{pmatrix} -\Re(H^2) & \Im(H^2) \\ -\Im(H^2) & -\Re(H^2) \end{pmatrix} \begin{pmatrix} \mathbf{q} \\ \mathbf{p} \end{pmatrix} \\ &= \Omega^2 \begin{pmatrix} \mathbf{q} \\ \mathbf{p} \end{pmatrix} \end{aligned} \quad (21)$$

in the form of Eq. (11) for real symmetric (Hermitian) matrix Ω^2 constructed from the real and imaginary parts of H^2 . The mapping of q and p to mechanical oscillators then follows from §II A 2.

For complex $N \times N$ Hamiltonian, there are thus most generally $2N$ mutually coupled oscillators. There can be fewer oscillators and no mutual coupling between specific oscillators, depending on the structure of H . As will be seen later, non-commuting rotations that comprise the operator Ω derived from H are directly related to the couplings. The displacements \mathbf{q} and \mathbf{p} provide an exact one-to-one mapping to the real and imaginary components, respectively, of the quantum state $|\Psi\rangle$. According to Eq. (21), the imaginary part of H^2 generates the coupling between these components. The state $\mathbf{c}(0) = \mathbf{q}(0) + i\mathbf{p}(0)$ uniquely determines the initial displacements, with the initial velocities then given by Eq. (20).

For real $H = Q$, $P = 0$, the present treatment gives the result in [30],

$$\ddot{\mathbf{q}} = -H^2 \mathbf{q} \quad (22)$$

and $\ddot{\mathbf{p}} = -H^2 \mathbf{p}$. Under this condition, \mathbf{q} and \mathbf{p} are conjugate variables (but are not most generally so) which evolve independently according to the same propagator, with no mechanical coupling between q and p oscillators. The initial conditions are the only difference in the solutions. One only needs a single set of N oscillators set in motion with two different sets of initial conditions to infer the quantum state $|\Psi\rangle$. Calculating $\mathbf{p} = H^{-1}\dot{\mathbf{q}}$ as in [30] imposes an additional unnecessary restriction that H , already constrained in [30] to be real, must be invertible (i.e., no eigenvalues equal to zero).

3. Extension to mixed states

The results in [30] and extensions in the previous section are limited to pure states evolving according to the Schrödinger equation. The methodology would appear to be inapplicable to mixed states. A statistical mixture can not be represented in terms of a state $|\Psi\rangle$, but is written in terms of the probability p_k for being in each of the possible states $|\Psi_k\rangle$, which defines a density matrix

$$\rho(t) = \sum_k p_k |\Psi_k(t)\rangle \langle \Psi_k(t)| \quad (23)$$

that evolves according to Liouville Eq. (2). It is an average over the \mathcal{N} constituents comprising a macroscopic system, which can be astronomically large, precluding an exact determination of the exact state of each of the \mathcal{N} constituents.

However, the density matrix representing a given system is not unique. The identical density matrix can also be constructed from a completely specified set of $N \ll \mathcal{N}$ noninteracting pure states, with the N^2 elements of ρ determined from measurable macroscopic (average) properties of the system, such as energy or polarization. In that case, both the weights p_k and corresponding states are known exactly, so each $|\Psi_k\rangle$ can be used independently to construct a set of coupled oscillators representing the components $c_i^{(k)}(t)$ of

$|\Psi_k(t)\rangle$. Rather than calculating density matrix evolution as $\rho(t) = U\rho(0)U^\dagger$, the simpler and more efficient Schrödinger evolution $|\Psi(t)\rangle = U|\Psi(0)\rangle$ can be applied to each pure state $|\Psi_k\rangle$ comprising ρ in Eq. (23). Subsequently, the weights p_k can be used to calculate expectation values, measurement probabilities, or reconstruct the density matrix at later times t if desired.

In addition, as shown in [34], at least one of the $|\Psi_k\rangle$ comprising the initial density matrix is redundant and can be removed from the calculation, since it provides a relatively uninteresting constant contribution to the system dynamics. Choose one of the weights, for example, p_1 . The density matrix can be rewritten as p_1 times the identity element plus a “pseudo” density matrix constructed from the $|\Psi_k\rangle$ with weights $(p_k - p_1)$. The term that is proportional to the identity element doesn’t evolve in time under unitary transformations and can be ignored.

Thus, the state $|\Psi_1\rangle$ has been removed from the density matrix, along with any other $|\Psi_k\rangle$ that had original weights $p_k = p_1$. In the general case of $m \geq 1$ degenerate statistical weights p_k , only $N - m$ of the $|\Psi_k\rangle$ are required. The number of oscillators is correspondingly reduced to $2N(N - m)$ resulting from $2N$ components for each $|\Psi_k\rangle$ and $N - m$ individual $|\Psi_k\rangle$. Choosing the weight with the largest degeneracy provides the maximum reduction. Unless the degeneracy is sufficiently large, $m > N/2$, this requires more oscillators than the maximum N^2 needed using the standard Liouville approach. However, the explicit contribution of each pure state to the system dynamics is readily apparent in applying this extended Schrödinger approach to the density matrix, providing an option for further insight. The density matrix at any given time is easily reconstructed as described in [34].

III. DISSIPATIVE SYSTEMS

The modifications necessary to model open systems as a set of damped oscillators can be found very generally using the Liouville representation, with minimal detail concerning the relaxation formalism. The Wangsness-Bloch equation expressing the evolution of the density operator in the presence of relaxation adds a relaxation operator term to Eq. (2) that operates on the density matrix [3, 35]. Expanding ρ in a basis of orthonormal operators as in Eq. (5) gives the real equation

$$\dot{\mathbf{r}} = \Omega \mathbf{r} + R \mathbf{r} + F(\mathbf{r}_{eq}). \quad (24)$$

The relaxation matrix R must be symmetric for relaxation elements that act symmetrically between states of the system, with diagonal elements providing auto-relaxation rates and off-diagonal elements giving cross-relaxation. The term F is a constant vector incorporating the asymptotic decay of the system to the steady state as a function of the equilibrium state \mathbf{r}_{eq} . Without this term, the solution decays to zero.

Differentiating again gives

$$\begin{aligned}\ddot{\mathbf{r}} &= (\Omega + R)\dot{\mathbf{r}} \\ &= \Omega[(\Omega + R)\mathbf{r} + F] + R\dot{\mathbf{r}},\end{aligned}\quad (25)$$

ie, a set of coupled oscillators with a velocity-dependent friction term and a constant applied force ΩF . A constant force in the harmonic oscillator equation merely shifts the origin of the coordinates. However, the matrix multiplying \mathbf{r} , which determines the mechanical couplings as given in Eq. (16), is no longer symmetric due to the sum of antisymmetric Ω and symmetric R , resulting in non-reciprocal off-diagonal couplings.

The precise role of non-reciprocal couplings in a classical model for quantum dissipative systems can be clarified by eliminating $\dot{\mathbf{r}}$ to obtain

$$\begin{aligned}\ddot{\mathbf{r}} &= (\Omega + R)^2\mathbf{r} + (\Omega + R)F \\ &= \Gamma^2\mathbf{r} + \Gamma F,\end{aligned}\quad (26)$$

a set of ideal (frictionless) coupled oscillators subjected to a constant applied force. In this case, however, the matrix Γ^2 is the sum of symmetric $\Omega^2 + R^2$ and antisymmetric $\Omega R + R\Omega$. The former term corresponds to a set of undamped oscillators with symmetric couplings $k_{ij} = k_{ji}$ (§II A 2), modified in comparison to no relaxation by inclusion of R^2 . The normal-mode frequencies are also modified accordingly.

Damping is provided by the antisymmetric part of Γ^2 , which gives antisymmetric couplings $\gamma_{ij} = -\gamma_{ji}$ and total coupling $\mathcal{K}_{ij} = k_{ij} + \gamma_{ij}$. The γ_{ij} therefore represent couplings connected in parallel with the symmetric k_{ij} and can be implemented, in principle, using magnetic materials and magnetic fields. For a given positive γ_{ij} , a positive displacement of mass m_j results in a positive force on m_i (using terms related to the schematic of Fig. 1). The resulting positive displacement of m_i provides a negative force on m_j due to $\gamma_{ji} < 0$ which opposes the original displacement of m_j and damps the motion. Stated differently, energy transferred from m_j to m_i is not reciprocally transferred back from m_i to m_j , and the motion is quenched. An antisymmetric coupling acts as a negative feedback mechanism that curbs system oscillations.

Equation (24) is typically written in the form of a homogeneous equation [3]. The inhomogeneous term F can be included in an augmented matrix $\tilde{\Gamma}$ formed by appending the vector F as a column to the right of Γ and then adding a correspondingly expanded row of zeros at the bottom. The vector \mathbf{r} is then augmented by including a last element equal to one to obtain the equivalent homogeneous equation

$$\frac{d^2}{dt^2}\tilde{\mathbf{r}} = \tilde{\Gamma}^2\tilde{\mathbf{r}}. \quad (27)$$

This is equivalent to appending the column ΓF to Γ^2 in Eq. (26), along with the associated row of zeros. The asymmetry of $\tilde{\Gamma}^2$ generates unphysical couplings that are not a problem theoretically but would preclude a real,

physical model. However, $\tilde{\Gamma}^2$ is readily written as the sum of symmetric $\tilde{\Gamma}_S^2 = \frac{1}{2}[\tilde{\Gamma}^2 + (\tilde{\Gamma}^2)^\dagger]$ and antisymmetric $\tilde{\Gamma}_A^2 = \frac{1}{2}[\tilde{\Gamma}^2 - (\tilde{\Gamma}^2)^\dagger]$, which determine the symmetric couplings k_{ij} and antisymmetric couplings γ_{ij} , respectively, as above.

In comparison, the Schrödinger equation can only include relaxation in certain special cases amenable to complex energies in the Hamiltonian. A typical application is the coupling between stable and unstable states and the resulting lifetimes of the states. An example relating velocity-dependent damping of classical oscillators to a Schrödinger equation treatment was provided in [30] in the weak-coupling limit. However, neither this approximation nor the required complex energies can be applied more generally. Even a simple two-level system with relaxation dynamics described by the Bloch equation cannot be addressed by the Schrödinger equation and requires the density matrix approach.

IV. REPRESENTATIVE EXAMPLES

Simple two-level systems are used as a prototype for implementing the quantum-classical mapping. Although they are already known to be representable by classical rotations in three-dimensional physical space, they provide sufficient detail to clarify the connection between real rotations of N -level quantum states in (i) $N^2 - 1$ dimensions (Liouville equation) or (ii) $2N$ dimensions (Schrödinger equation) and their mapping to (i) $N^2 - 1$ or (ii) $2N$ classical oscillators in one-dimensional physical space. The actual number of oscillators needed can be less, depending on the structure of the specific Hamiltonian, as illustrated in the examples provided. In what follows, vectors written for convenience as rows in the text are to be understood as column vectors when used in matrix equations.

A. Closed systems (unitary time evolution)

1. Quantum solution

In terms of real Δ_1, Δ_2 and complex $V = \omega_1 - i\omega_2$, the Hamiltonian for a general 2-level system can be written in terms of the Pauli matrices σ_i ($i = 1, 2, 3$) and $\sigma_0 = \mathbb{1}$ as

$$H = \begin{pmatrix} \Delta_1 & V \\ V^* & \Delta_2 \end{pmatrix} = \sum_{\alpha=0}^3 \omega_\alpha \sigma_\alpha, \quad (28)$$

with $\omega_0 = (\Delta_1 + \Delta_2)/2$ and $\omega_3 = (\Delta_1 - \Delta_2)/2$. The σ_0 term commutes with the other terms, so the propagator $U(t) = e^{-iHt}$ giving the Schrödinger equation solution as in Eq. (17) is readily obtained in terms of $\omega_i \sigma_i$ ($i = 1, 2, 3$). The standard expansion of $e^{-i\boldsymbol{\omega} \cdot \boldsymbol{\sigma} t}$ using unit

vector $\hat{\omega} = \omega/\omega$ gives

$$\begin{aligned} U(t) &= e^{-i\omega_0 t} e^{-i\omega \cdot \sigma} \\ &= e^{-i\omega_0 t} [\cos \omega t - i \hat{\omega} \cdot \sigma \sin \omega t] \\ &= e^{-i\omega_0 t} \begin{pmatrix} a & b \\ -b^* & a^* \end{pmatrix}. \end{aligned} \quad (29)$$

The parameters a, b obtained from expanding $\hat{\omega} \cdot \sigma$ and using the matrix forms for the σ_i are

$$\begin{aligned} a &= \cos \omega t - i \hat{\omega}_3 \sin \omega t \\ b &= -(\hat{\omega}_2 + i \hat{\omega}_1) \sin \omega t, \end{aligned} \quad (30)$$

recognizable from classical mechanics as the Cayley-Klein parameters for a rotation by angle $2\omega t$ about $\hat{\omega}$.

Evolution of the Schrödinger state $|\Psi\rangle \leftrightarrow (c_1, c_2)$ proceeds according to Eq. (17), with the corresponding density matrix states $\rho_{ij} = c_i c_j^*$ evolving according to Eq. (3). The equivalent classical evolution is considered next.

2. Classical representation (Liouville equation)

Using the σ_α as the basis and inner product $\langle \sigma_\alpha | \sigma_\beta \rangle = 1/2 \text{Tr}(\sigma_\alpha \sigma_\beta) = \delta_{\alpha\beta}$ gives $\Omega_{0\alpha} = 0 = \Omega_{\alpha 0}$ according to Eq. (8). The remaining 3×3 matrix giving the non-zero couplings is easily determined using the commutation relations $[\sigma_i, \sigma_j] = 2i \epsilon_{ijk} \sigma_k$ written in terms of the usual Levi-Civita tensor ϵ_{ijk} (equal to ± 1 for cyclic/anticyclic permutations of the indices $j, k, l = 1, 2, 3$ and zero otherwise) summed over repeated indices for slightly more concise notation. Then

$$\begin{aligned} \Omega_{ij} &= \langle [\sigma_i, \sigma_j] | H \rangle \\ &= -2\epsilon_{ijk} \langle \sigma_k | \omega \cdot \sigma \rangle \\ &= -2\omega_l \epsilon_{ijk} \langle \sigma_k | \sigma_l \rangle \\ &= -2\omega_k \epsilon_{ijk} \\ \Omega &= 2 \begin{pmatrix} 0 & -\omega_3 & \omega_2 \\ \omega_3 & 0 & -\omega_1 \\ -\omega_2 & \omega_1 & 0 \end{pmatrix}. \end{aligned} \quad (31)$$

Four coupled oscillators are needed to represent $(q_1, q_2, p_1, p_2) \equiv (r_1, r_2, r_3, r_4)$. The mutual couplings k_{ij} ($i \neq j$) given by Eq. (16) are the corresponding elements

The resulting equation of motion

$$\dot{\mathbf{r}} = \Omega \mathbf{r} = 2\omega \times \mathbf{r} \quad (32)$$

represents a rotation of \mathbf{r} about axis $\omega = (\omega_1, \omega_2, \omega_3)$ at angular frequency 2ω , as expected from the FVH Theorem for arbitrary two-level systems. However, the equivalence of quantum dynamics, in the case of 2-level systems, to a rotation in real, physical space cannot be generalized to arbitrary N-level systems. Representing quantum dynamics by a system of coupled harmonic oscillators in one physical dimension is general for any value of N .

The coupling matrix is

$$\Omega^2 = 4 \begin{pmatrix} -(\omega_2^2 + \omega_3^2) & \omega_1 \omega_2 & \omega_1 \omega_3 \\ \omega_1 \omega_2 & -(\omega_1^2 + \omega_3^2) & \omega_2 \omega_3 \\ \omega_1 \omega_3 & \omega_2 \omega_3 & -(\omega_1^2 + \omega_2^2) \end{pmatrix}, \quad (33)$$

giving three mutually coupled oscillators as in Fig. 1. The couplings obtained from Eq. (16) are

$$\begin{aligned} k_{ij}/4 &= \omega_i \omega_j \quad i \neq j \\ k_{ii}/4 &= \omega_j^2 + \omega_k^2 - \omega_i \omega_j - \omega_i \omega_k \quad i \neq j \neq k \\ &= \omega_j(\omega_j - \omega_i) + \omega_k(\omega_k - \omega_i). \end{aligned} \quad (34)$$

Unless two components of ω are zero, any possible ordering for the relative magnitudes of these components makes at least one of the k_{ii} negative, assuming all components of ω are positive. Alternatively, $k_{ij} < 0$ if $\omega_i < 0$ and $\omega_j > 0$. Either way, negative couplings are a required feature of the quantum-classical mapping.

3. Classical Representation (Schrödinger equation)

The matrix Ω leading to a solution for (\mathbf{q}, \mathbf{p}) as a rotation $e^{-\Omega t}$ of the initial state $(\mathbf{q}_0, \mathbf{p}_0)$ is comprised of the real and imaginary parts of H as in Eq. (20), giving

$$\Omega = \begin{pmatrix} 0 & \omega_2 & \Delta_1 & \omega_1 \\ -\omega_2 & 0 & \omega_1 & \Delta_2 \\ -\Delta_1 & -\omega_1 & 0 & \omega_2 \\ -\omega_1 & -\Delta_2 & -\omega_2 & 0 \end{pmatrix} \quad (35)$$

and coupling matrix

$$\Omega^2 = \begin{pmatrix} -\Delta_1^2 - (\omega_1^2 + \omega_2^2) & -\omega_1(\Delta_1 + \Delta_2) & 0 & -\omega_2(\Delta_1 + \Delta_2) \\ -\omega_1(\Delta_1 + \Delta_2) & -\Delta_2^2 - (\omega_1^2 + \omega_2^2) & \omega_2(\Delta_1 + \Delta_2) & 0 \\ 0 & \omega_2(\Delta_1 + \Delta_2) & -\Delta_1^2 - (\omega_1^2 + \omega_2^2) & -\omega_1(\Delta_1 + \Delta_2) \\ -\omega_2(\Delta_1 + \Delta_2) & 0 & -\omega_1(\Delta_1 + \Delta_2) & -\Delta_2^2 - (\omega_1^2 + \omega_2^2) \end{pmatrix}. \quad (36)$$

of Ω^2 . The self-couplings for $i = 1, 2$ are

$$k_{ii} = \Delta_i^2 + \omega_1^2 + \omega_2^2 - (\omega_1 + \omega_2)(\Delta_1 + \Delta_2), \quad (37)$$

with $k_{33} = k_{11}$ and $k_{44} = k_{22}$. Negative couplings are required in general.

The operator Ω generates simultaneous rotations in the planes (r_i, r_j) associated with the nonzero Ω_{ij} . The nonzero mutual couplings in Ω^2 represent noncommuting rotations in Ω . One easily shows that noncommuting rotations share a common coordinate axis in their respective rotation planes, such as (r_2, r_1) and (r_1, r_3) . Then $\Omega_{21}\Omega_{13} = (\Omega^2)_{23}$ gives a nonzero mutual coupling k_{23} . A rotation in the (r_1, r_2) plane *does* commute with a rotation in the (r_3, r_4) plane, so one expects the mapping from rotations to oscillators to generate at least one mutual coupling equal to zero in this case. For the particular example here, the structure of Ω is such that $(\Omega^2)_{13} = 0 = (\Omega^2)_{24}$, giving zero for k_{13} and k_{24} . Mass 1 is not coupled to mass 3, and mass 2 is not coupled to mass 4. Similarly, elements Ω_{ij} that equal zero (signifying no rotation in the (r_i, r_j) -plane) make no contribution to couplings k_{il} or k_{lj} , which may be zero, depending on the other elements of Ω .

4. Quantum dimer

The quantum dimer example provided in [30] corresponds to real $V = \omega_1$, with $\omega_2 = 0$, and $\Delta_1 = \Delta_2 = \omega_0$, giving $\omega_3 = 0$.

a. Liouville approach The only nonzero elements of Ω in Eq. (31) are then $\Omega_{32} = 2V = -\Omega_{23}$, leading to diagonal entries $(\Omega^2)_{22} = (\Omega^2)_{33} = -4V^2$ as the only nonzero elements of Ω^2 in Eq. (34). Thus, only two uncoupled oscillators, each with natural frequency $2V$, are needed to represent this particular quantum system, as opposed to the maximum limit of three. The initial conditions determine the specific details of the time evolution.

For $\Psi(t) = [c_1(t), c_2(t)]$ and initial condition $\Psi(0) = (1, 0)$, as in [30], one easily obtains $\mathbf{r}(0) = (0, 0, 1/2)$ using $r_i = 1/2\text{Tr}(\sigma_i \rho)$, resulting in $\dot{\mathbf{r}}(0) = [0, -V, 0]$ from Eq. (32). Then

$$\mathbf{r}(t) = \frac{1}{2} \begin{pmatrix} 0 \\ -\sin 2Vt \\ \cos 2Vt \end{pmatrix}, \quad (38)$$

which is the expected rotation about axis $\hat{\omega} = \hat{\omega}_1$ at angular frequency $2\omega_1 t = 2Vt$ given by Eq. (30). Since the two oscillators are out of phase by 90° , the system can actually be represented by a single oscillator—the position of one oscillator automatically gives the position of the other from a simple phasor diagram.

b. Schrödinger approach Referring to the 2×2 block structure of Ω^2 in Eq. (36), one finds off-diagonal blocks equal to zero, since they depend on ω_2 , the imaginary part of V . The two remaining nonzero blocks on the diagonal generate independent evolution of \mathbf{q} and \mathbf{p} . The \mathbf{q} -block gives two coupled oscillators with mutual coupling $k_{12} = -2\omega_0 V$ and self-couplings $k_{ii} = (\omega_0 - V)^2$ from Eq. (37). The \mathbf{p} -block gives identical couplings.

One can instead switch to a positive value for the mutual coupling, as in [30], since changing the sign of V only interchanges the normal-mode eigenvalues $-(\omega_0 \pm V)^2$ of Ω^2 . This changes the sense of rotation generated by H in Hilbert space and hence, by Ω in the real 4-dimensional space. Using a positive coupling in this way captures the essential elements of the problem, but does not, strictly speaking, faithfully map the quantum system to the oscillator system. There are relatively few cases where negative couplings can be finessed away in this fashion.

With the definitions in §II B 1, the initial condition $\mathbf{c}(0) = (1, 0)$ corresponds to $(\mathbf{q}_0, \mathbf{p}_0) = (1, 0, 0, 0)$, which extracts the first column of Ω in the matrix multiplication of Eq. (20) to give $(\dot{\mathbf{q}}_0, \dot{\mathbf{p}}_0) = (0, 0, -\omega_0, -V)$. The four oscillators must be set in motion with these initial conditions for their displacements in a mechanical implementation to correspond to the evolution of $|\Psi(t)\rangle = [c_1(t), c_2(t)]$.

However, a solution for the motion requires only the initial displacements. The propagator $U(t)$ is readily obtained from Eq. (14) in terms of the eigenvectors $(1, 1)$ and $(1, -1)$ for each 2×2 block on the diagonal, padded with zeros to give the appropriate four-element vector. The given initial condition picks out the first column of $U(t)$ to reproduce the solution given in [30]. The Schrödinger equation requires four coupled oscillators for this particular example, in contrast to two uncoupled oscillators for the Liouville representation (equivalent to a single oscillator, since they are always 90° out of phase).

5. Symmetric unperturbed levels

Consider $\Delta_1 = -\Delta_2 = \omega_3$, which arises in representing two unequal energy levels relative to the mean energy of the levels.

a. Liouville approach There are no nonzero elements of Ω^2 derived from Eq. (33). The system is fully coupled, as illustrated in Fig. 1, and represents the most general result for this approach. The Schrödinger approach, discussed next, provides a simpler representation in this case.

b. Schrödinger approach The matrix Ω^2 of Eq. (36) is now diagonal for any general complex perturbation V . Four uncoupled oscillators, each with natural frequency $(\sum_i \omega_i^2)^{1/2}$, represent the system. Specifying $|\Psi(0)\rangle$ determines the initial conditions as discussed previously. This is a very simple system, with each oscillator evolving independently.

The Liouville approach, by contrast, results in a relatively more complex system, albeit with one less oscillator. Yet, for the dimer example, the Liouville implementation is much simpler than the Schrödinger implementation. Which approach gives the simpler set of oscillators and couplings depends on the specific problem.

B. Open (dissipative) systems

1. Bloch equation with relaxation

The solution of the Bloch equation for the time dependence of nuclear magnetization in a magnetic field is relatively simple for a field along the z -axis [36]. As is well-known, the transverse magnetization precesses about the field at the Larmor frequency while decaying exponentially at a transverse relaxation rate $1/T_2$. The longitudinal magnetization relaxes to the equilibrium magnetization at a rate $1/T_1$. The mapping of this motion to a system of damped oscillators illustrates the procedure described in §III, as well as the role of non-reciprocal couplings in the model.

The inhomogeneous term F in Eq. (24) is $(0, 0, M_0/T_1)$, where M_0 is the equilibrium magnetization. Vector \mathbf{r} represents the nuclear magnetization. Denoting ω_3 as the Larmor frequency, the matrix $\Gamma = \Omega + R$ is

$$\Gamma = \begin{pmatrix} -\frac{1}{T_2} & -\omega_3 & 0 \\ \omega_3 & -\frac{1}{T_2} & 0 \\ 0 & 0 & -\frac{1}{T_1} \end{pmatrix}. \quad (39)$$

As described earlier, appending a column ΓF to the right of Γ^2 followed by a row of zeros at the bottom gives Eq. (27) for the oscillator equation, with

$$\tilde{\Gamma}^2 = \begin{pmatrix} \frac{1}{T_2} - \omega_3^2 & \frac{2\omega_3}{T_2} & 0 & 0 \\ -\frac{2\omega_3}{T_2} & \frac{1}{T_2} - \omega_3^2 & 0 & 0 \\ 0 & 0 & \frac{1}{T_1^2} & -\frac{M_0}{T_1^2} \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad (40)$$

and $\tilde{r}_4 = 1$ augmenting \mathbf{r} to represent a static component that incorporates the inhomogeneous term ΓF . The necessary couplings are easily read from symmetric Γ_S^2 and antisymmetric Γ_A^2 that sum to give $\tilde{\Gamma}^2$:

$$\begin{aligned} \tilde{\Gamma}_S^2 &= \begin{pmatrix} \frac{1}{T_2} - \omega_3^2 & 0 & 0 & 0 \\ 0 & \frac{1}{T_2} - \omega_3^2 & 0 & 0 \\ 0 & 0 & \frac{1}{T_1^2} & -\frac{M_0}{2T_1^2} \\ 0 & 0 & -\frac{M_0}{2T_1^2} & 0 \end{pmatrix} \\ \tilde{\Gamma}_A^2 &= \begin{pmatrix} 0 & \frac{2\omega_3}{T_2} & 0 & 0 \\ -\frac{2\omega_3}{T_2} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{M_0}{2T_1^2} \\ 0 & 0 & \frac{M_0}{2T_1^2} & 0 \end{pmatrix}. \end{aligned} \quad (41)$$

A symmetric coupling $k_{34} = -M_0/(2T_1^2)$ connected in parallel with antisymmetric (nonreciprocal) coupling $\gamma_{34} = -M_0/(2T_1^2)$ provides the contribution to the final steady state magnetization \tilde{r}_3 through coupling to \tilde{r}_4 . The vanishing of $k_{43} + \gamma_{43}$ ensures there is no coupling from \tilde{r}_3 to change the static component \tilde{r}_4 . Although there is no friction term in Eq. (27), the mechanism that damps \tilde{r}_3 is fairly transparent. Since $k_{31} = 0 = k_{32}$,

\tilde{r}_3 is only coupled to static \tilde{r}_4 , which effectively shifts \tilde{r}_3 to $z = \tilde{r}_3 - M_0$, giving the equivalent equation $\ddot{z} = z/T_1^2$. The self-coupling k_{33} is the source of the imaginary natural frequency i/T_1 , resulting in the standard damped solution $z(t) = z(0)e^{-t/T_1}$.

The mechanism for transverse relaxation is perhaps more interesting, given that the diagonal elements $\tilde{\Gamma}_{ii}^2$ ($i = 1, 2$) cannot be the source of the damping for the case $\omega_3 = 1/T_2$. Since $\tilde{\Gamma}_{11}^2 = \tilde{\Gamma}_{22}^2$, the eigenvalues of $\tilde{\Gamma}^2$ are $\tilde{\Gamma}_{11}^2$ plus the eigenvalues for the antisymmetric block, which are $\pm 2i\omega_3/T_2$ (compared to $\pm 2\omega_3/T_2$ for symmetric couplings). The normal mode frequencies, given by the square root of the eigenvalues, are $\omega_3 \pm i/T_2$. When $\tilde{\Gamma}_{11}^2 = 0$, the antisymmetric coupling is the sole source of the imaginary frequency producing the required e^{-t/T_2} decay of the transverse magnetization.

V. SYSTEM INVARIANTS

Dynamical variables that are known to be constant in time can provide insight into the behavior of dynamical processes. They are particularly useful when a solution for the time evolution is not available. The invariants for quantum N-level systems can be classified in three categories. The most general category depends only on the initial state of the system. These invariants are independent of the system Hamiltonian and the propagator for the time evolution of the system states. Since this evolution is a rotation, this class of invariants provides information on the space of accessible states under any possible rotation of a given initial state.

The next level of invariant requires input from the system Hamiltonian and provides further information on the subspace of states accessible under particular rotations. The final category requires the Hamiltonian and normal modes for the system, which is input that is also sufficient to calculate the propagator. Although the accessible state space can then be explicitly determined, this class of invariants still provides potentially useful symmetry laws for a given dynamical system.

A. Hamiltonian-independent invariants

For an N-level system, $\text{Tr}(\rho^n)$ is known to provide as many as $n \leq N$ independent invariants [5] (and also [6] for $N = 3$). Although the relation applies equally well to both pure and mixed states, $\rho^n = \rho$ for a pure state, so for this case the conservation law only gives a single invariant which merely expresses the conservation of probability, $\text{Tr}(\rho) = 1$.

B. Hamiltonian-dependent invariants

1. Real rotations

The energy of the oscillator system provides a very general invariant applicable to either pure or mixed states, but it is dependent on H . Differentiating Eq. (9) gives $\ddot{\mathbf{r}} = \Omega \dot{\mathbf{r}}$, leading to Eq. (11). The solution $\dot{\mathbf{r}} = e^{\Omega t} \dot{\mathbf{r}}(0)$ is a rotation, so the magnitude or norm $\|\dot{\mathbf{r}}\|$ of vector $\dot{\mathbf{r}}$ is constant, along with $\|\mathbf{r}\|$.

Thus, for oscillators representing real rotations, the total kinetic energy $T = 1/2 \|\dot{\mathbf{r}}\|^2$ of the oscillator system is conserved. This could be anticipated, since there is only rotational energy prior to the oscillator mapping. The potential energy $U = -1/2(\Omega^2)_{ij} r_i r_j$ must therefore also be related to T . Writing U in matrix form and using $\Omega^2 = -\Omega^\dagger \Omega$ together with $\langle r | \Omega^\dagger = \langle \Omega r | = \langle \dot{r} |$ gives

$$U = -\frac{1}{2} \langle r | \Omega^2 r \rangle = \frac{1}{2} \langle \Omega r | \Omega r \rangle = T \quad (42)$$

at all times, resulting in total energy $2T$. This can be compared with the virial theorem for the average values $\langle T \rangle = -1/2 \langle \mathbf{F} \cdot \mathbf{r} \rangle$, noting that the force $\mathbf{F} = \Omega^2 \mathbf{r}$ gives $\langle U \rangle$, and the averages are the same as the constant values.

Comparing states of the same norm, the system cannot evolve to a state $\mathbf{r}(t)$ from an initial state $\mathbf{r}(0)$ if it fails to conserve the energy $E = \|\dot{\mathbf{r}}\|^2 = \|\Omega \mathbf{r}\|^2$ of the initial configuration. On the other hand, a state that is allowed energetically is not necessarily accessible. Most simply, reflecting $\mathbf{r}(0)$ through the origin results in states $-\mathbf{r}(t)$ that conserve $\|\Omega \mathbf{r}\|$ but are not accessible solutions for the time evolution of $\mathbf{r}(0)$, which is expressed as a rotation.

More generally, differentiating Eq. (9) any number of times gives

$$\|(d/dt)^n \mathbf{r}(t)\| = \|\Omega^n \mathbf{r}(t)\| = \|\Omega^n \mathbf{r}(0)\|. \quad (43)$$

They are not independent, but are included for completeness. They provide unique information only for a single value of n .

2. Hilbert space rotations

For $\mathbf{r} \rightarrow \mathbf{c}$ and $\Omega \rightarrow -iH$, the analysis of the previous section gives

$$\|H^n \mathbf{c}(t)\| = \|H^n \mathbf{c}(0)\| \quad (44)$$

starting with Eq. (19). Although complex rotations can be transformed into real rotations as discussed in §II B, Eq. (44) can be used more directly to characterize accessibility in the Schrödinger state space. As before, the invariants are not independent, and $n = 1$ would typically be the simplest choice. A violation of any invariant renders a state inaccessible. These invariants are also related

to conservation of energy, since $\|H^n \mathbf{c}\|^2 = \langle c | H^n H^n | c \rangle$, the expectation value of H^{2n} for the given state.

Consider the extension of the quantum dimer example of [30] to three coupled monomers such as atoms or molecules that each have only a ground state and one excited state of energy ω_0 . For a linear array and only nearest neighbor interactions ω_1 ,

$$H = \begin{pmatrix} \omega_0 & \omega_1 & 0 \\ \omega_1 & \omega_0 & \omega_1 \\ 0 & \omega_1 & \omega_0 \end{pmatrix}. \quad (45)$$

It is immediately clear from the structure of H that if the system starts in the state $(1, 0, 0)$, complete transfer to the state $(0, 1, 0)$ is not possible, since $\|H\mathbf{c}\|^2$ is $\omega_0^2 + \omega_1^2$ initially and $\omega_0^2 + 2\omega_1^2$ in the final state. In fact, transfer to any (normalized) state of the form $(0, a, b)$ is not allowed, while complete transfer from the initial state to $(0, 0, 1)$ cannot be ruled out. As an aside, the matrix $\omega_0 \mathbb{1}$ obviously commutes with the rest of H , so it merely contributes a global phase $e^{-i\omega_0 t}$ to the solution which can be set equal to zero.

For a circular array, monomers one and three are also nearest neighbors, so $H_{13} = \omega_1 = H_{31}$ instead of zero as in Eq. (45). Complete transfer out of monomer one as above from $(1, 0, 0)$ to $(0, a, b)$ is allowed only for $a = 0$ or $b = 0$. Transfer to the states $(0, 1, 0)$ or $(0, 0, 1)$ are therefore allowed, but are not necessarily in the solution space.

C. Normal-mode-dependent invariants

Although transforming Eq. (11) to normal coordinates $\boldsymbol{\eta}$ is equivalent to finding the solution $\mathbf{r}(t)$ for the state vector, as in Eq. (14), the correspondence between real rotations and coupled oscillators provides additional invariants for N-level systems derived from the normal modes of the oscillators.

As is well known, a real antisymmetric matrix, such as Ω , has imaginary eigenvalues that appear in conjugate pairs, $\pm i\lambda_i$. In the odd-dimension case, there is an additional eigenvalue equal to zero. Every such Ω can also be made block-diagonal by an orthogonal transformation. The transformed matrix consists of antisymmetric 2×2 blocks with (real) elements $\pm \lambda_i$. The equivalence of a rotation generated by Ω to a system of coupled oscillators represented by Ω^2 provides a bridge to a normal mode analysis of system dynamics.

Since Ω^2 is hermitian, there is a basis consisting of its orthonormal eigenvectors. If the similarity transformation, T , that diagonalizes Ω^2 is constructed from these orthonormal eigenvectors, then $T^\dagger \Omega^2 T = \tilde{\Omega}^2$ is also the transformation that makes $T^\dagger \Omega T = \tilde{\Omega}$ block-diagonal. This is the specific square root of $\tilde{\Omega}^2$ (out of many) that can be inverse-transformed to the generator of the rotation, Ω . The nonzero antisymmetric elements $\tilde{\Omega}_{ij} = -\tilde{\Omega}_{ji}$ in this normal mode basis are the real terms,

$\pm\lambda_i$, in the eigenvalues $\pm i\lambda$ of Ω . Since the operator $\tilde{\Omega}$ generates a rotation according to the equation $\dot{\boldsymbol{\eta}} = \tilde{\Omega}\boldsymbol{\eta}$, the $\tilde{\Omega}_{ij}$ are the angular frequencies for rotations of $\boldsymbol{\eta}(t)$ in planes (η_i, η_j) . Furthermore, the 2×2 block-diagonal structure of $\tilde{\Omega}$ ensures that nonzero elements $\tilde{\Omega}_{ij}$ in different blocks share no common indices. The rotations generated by each block therefore commute, since non-commuting rotations in planes (η_i, η_j) share a common coordinate axis, as mentioned in §IV A 3.

The diagonalized matrix $\tilde{\Omega}^2$ then consists of pairs of degenerate eigenvalues $(\tilde{\Omega}^2)_{ii}$ and $(\tilde{\Omega}^2)_{jj}$ equal to $-(\tilde{\Omega}_{ij})^2$. If the dimension of the real rotation space is odd, the one unpaired eigenvalue is equal to zero. The normal mode coordinate associated with this eigenfrequency is static and invariant. In addition, each rotation in a plane (η_i, η_j) maps to uncoupled oscillators at η_i and η_j with equal natural frequency $|\Omega_{ij}|$, but 90° out of phase. As a rotation, $\eta_i^2 + \eta_j^2$ is constant. Transforming from this normal-mode basis to the coordinate basis \mathbf{r} provides invariant dynamical variables that can be used to characterize the behavior of the given system.

More specifically, consider a rotation in three dimensions about an axis in the (r_1, r_3) -plane, represented by Ω from Eq. (31) with $\omega_2 = 0$ (and ignoring the scale factor 2 specific to the original example). Results from this simple example can almost be obtained by inspection, yet it illustrates fully the aspects of the more general discussion above. The evolution equation $\dot{\mathbf{r}} = \Omega\mathbf{r}$ drives simultaneous, noncommuting rotations in the (r_1, r_2) and (r_2, r_3) planes at frequencies ω_3 and ω_1 , respectively. The net rotation is about the axis $\boldsymbol{\omega} = (\omega_1, 0, \omega_3)$ at frequency $\omega = (\omega_1^2 + \omega_3^2)^{1/2}$. The transformation T which diagonalizes Ω^2 in Eq. (33) is a (right-hand) rotation of the coordinates about the r_2 axis by angle θ defined by $\tan \theta = \omega_1/\omega_3$. Transforming to normal coordinates gives

$$\boldsymbol{\eta} = T^\dagger \mathbf{r} = \begin{pmatrix} \cos \theta & 0 & -\sin \theta \\ 0 & 1 & 0 \\ \sin \theta & 0 & \cos \theta \end{pmatrix} \mathbf{r} \quad (46a)$$

$$\tilde{\Omega}^2 = T^\dagger \Omega^2 T = \begin{pmatrix} -\omega^2 & 0 & 0 \\ 0 & -\omega^2 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad (46b)$$

$$\tilde{\Omega} = T^\dagger \Omega T = \begin{pmatrix} 0 & -\omega & 0 \\ \omega & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \quad (46c)$$

Matrix $\tilde{\Omega}$ generates a rotation at frequency ω in the (η_1, η_2) plane which maps to the two uncoupled oscillators represented in Eq. (46b) of the same natural frequency, $\omega = \sqrt{-(\tilde{\Omega}^2)_{11}} = \sqrt{-(\tilde{\Omega}^2)_{22}}$. As a rotation, the magnitude of (η_1, η_2) is invariant. The zero-frequency oscillator given by $(\tilde{\Omega}^2)_{33}$ corresponds to the rotation axis η_3 in $\tilde{\Omega}$, which is also a system invariant. The transformation in Eq. (46a) gives the invariant dynamical variables

$$\begin{aligned} \eta_3 &= r_1 \sin \theta + r_3 \cos \theta \\ \eta_1^2 + \eta_2^2 &= (r_1 \cos \theta - r_3 \sin \theta)^2 + r_2^2, \end{aligned} \quad (47)$$

i.e., linear combinations of the $r_i(t)$ that are constant in time for any initial state $\mathbf{r}(0)$. These are distinct from excitation of standard vibrational modes such as $\eta_1 \neq 0$, $\eta_2 = 0 = \eta_3$, which give the usual invariants related to the decoupling of the normal modes.

VI. CONCLUSION

General N-level quantum systems can be represented as assemblies of classical coupled oscillators, with values for the classical coupling constants readily obtained from the system Hamiltonian. There is a direct one-to-one correspondence between the quantum states of the system and the oscillator positions. The formalism presented includes both closed and open (dissipative) systems. It provides the possibility for visual, mechanical insight into abstract quantum systems, as well as a metric for characterizing the interface between quantum and classical mechanics. Since the harmonic oscillator is the foundation for modeling a wide range of physical systems, these results might also be expected to have applications beyond their context here.

For closed systems represented by a density matrix, the known evolution of states as rotations of a single coherence vector in a real (but unphysical) hyperspace of $n = N^2 - 1$ dimensions [3, 5] has been mapped here to the evolution of n oscillators in one physical dimension. The evolution of Schrödinger states has also been generalized here to real rotations in $n = 2N$ dimensions, which can be mapped to n oscillators. In principle, n can be reduced to $2(N - 1)$ by the normalization condition and choice of a specific value (typically zero) for the arbitrary and physically meaningless global phase of the state vector [3]. Only $n = N$ oscillators are required if the Hamiltonian is real. The scaling of quantum systems to classical systems is thus linear for Schrödinger states rather than quadratic for density matrix representations.

The generator of each rotation can be represented as a linear combination of the generators for $\text{SO}(n)$, the group of rotations about a fixed point in n -dimensional Euclidean space, which does not appear to have been emphasized previously. The equivalence of real rotations and classical oscillators then provides further insight into system dynamics. The group generators represent separate rotations in orthogonal planes. Any of the individual orthogonal rotations in two dimensions maps to two independent oscillators, 90° out of phase. A rotation effected by a linear combination of generators maps to oscillators with couplings that represent the noncommuting rotations among the generators. In a sense, this provides a more general analogue, in reverse, to the well known mapping of one oscillator to a phasor rotation. The dynamics of coupled oscillators provide previously overlooked invariants (constants of the motion) for the rotations that represent the dynamics of N-level systems. In addition, both positive and negative couplings are required most generally.

Ideal, frictionless, classical coupled oscillators also provide an exact model for open systems. Dissipation is generated by antisymmetric couplings which emerge naturally as a result of extending the formalism to open systems.

The results are applicable to time-independent Hamiltonians, which is sufficiently general for a great many cases of practical interest. Time-dependent Hamiltonians (i.e., driven systems) can be approximated to a chosen level of accuracy by a sequence of constant Hamiltonians over sufficiently short time steps. Modeling a time-dependent quantum Hamiltonian as classical requires new spring constants (or their analogues) for the mechanical system at each time step, together with a reinitialization of the velocities derived from the new positions of the oscillators according to Eq. (9). By contrast, velocities in the natural dynamics of a system of coupled oscillators would not change discontinuously with a change in spring constants.

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Appendix: Weak coupling approximation

The form the exact results reduce to in the limit of weak system perturbations is considered here, generalizing the analysis for real H detailed in [30]. The topic is of some interest in the context of previous treatments of quantum-classical connections that assume weak coupling at the outset [22–29]. Exact and approximate expressions provide a quantitative comparison, enabling the accuracy and relevance of such approximations to be readily assessed.

If off-diagonal elements H_{ij} are sufficiently small compared to any of the diagonal elements, then ignoring products $H_{ij}H_{kl}$ of two off-diagonal elements in Eq. (22) (second-order terms) provides a good approximation to the exact results. Each $\ddot{q}_i = \sum_j -(H^2)_{ij}q_j$ is a linear combination of the q_j with coefficients $-H_{ik}H_{kj}$. The effect of the weak coupling approximation is to change the value of the coefficients as follows. Separating the $k = i$ term from the k summation, followed by writing the $j = i$ term separate from the j summation, then taking the $k = j$ term out of the remaining double sum gives

$$\begin{aligned}\ddot{q}_i &= -\sum_j (H^2)_{ij} q_j = -\sum_{j,k} H_{ik} H_{kj} q_j = -\sum_j \left[H_{ii} H_{ij} + \sum_{k \neq i} H_{ik} H_{kj} \right] q_j \\ &= -\left[H_{ii} H_{ii} + \sum_{k \neq i} H_{ik} H_{ki} \right] q_i - \sum_{j \neq i} \left[H_{ii} H_{ij} + \sum_{k \neq i} H_{ik} H_{kj} \right] q_j \\ &= -\left[H_{ii} H_{ii} + \sum_{k \neq i} H_{ik} H_{ki} \right] q_i - \sum_{j \neq i} \left[H_{ii} H_{ij} + H_{ij} H_{jj} \right] q_j - \sum_{j \neq i} \sum_{\substack{k \neq i \\ k \neq j}} H_{ik} H_{kj} q_j \\ \ddot{q}_i + \left[(H_{ii})^2 + \sum_{k \neq i} (H_{ki})^2 \right] q_i &= -\sum_{j \neq i} \left[(H_{ii} + H_{jj}) H_{ij} + \sum_{\substack{k \neq i \\ k \neq j}} H_{ik} H_{kj} \right] q_j,\end{aligned}\tag{A.1}$$

which is Eq. (21) of reference [30] after moving the q_i term included in a summation there to the left side of the equation and defining diagonal elements $H_{nn} \equiv \omega_n$. The substitution $H_{ik} = H_{ki}$ is used above, since H is real and Hermitian.

The sums over index k in Eq. (A.1) are clearly identifiable as second-order terms, while the coefficient involving a single sum over index j is a product of first-order H_{ij} and larger diagonal elements. Omitting second-order terms gives the result in the weak coupling approxima-

tion as

$$\ddot{q}_i + H_{ii}^2 q_i = -\sum_{j \neq i} (H_{ii} + H_{jj}) H_{ij} q_j.\tag{A.2}$$

Comparison with Eq. (A.1) shows the exact result merely modifies values for the natural frequency of the oscillator associated with position q_i and modifies the couplings to the other oscillators. Most generally, therefore, it causes no increase in the complexity of the calculation, so there would be no particular advantage to using the weak coupling approximation. On the other hand, in specific cases, the structure of the Hamiltonian may be

such that coupling coefficients of some coordinates become zero in the weak coupling approximation, which might simplify a given problem. The classical q -coupled equations used as a model for comparison to exact results in [30] lack the H_{jj} term in Eq. (A.2)—a further approximation that would be more difficult to justify, since the diagonal elements of H can't all be small relative to each other.

Extending the results considered here to complex H is straightforward. Equation (21) is of the form $\ddot{\mathbf{r}} =$

$\Omega^2 \mathbf{r}$, with real, symmetric Ω^2 and $\mathbf{r} = (\mathbf{q}, \mathbf{p})$. The weak coupling condition becomes $\Omega_{ij} \ll \Omega_{nn}$, which simply adds the requirement that the imaginary parts of H_{ij} also be sufficiently small compared to the diagonal elements. Then, in Eqs. (A.1,A.2), $q \rightarrow r$, and $H \rightarrow \Omega$.

Finally, the secular approximation, applied, for example, in perturbation theory, provides a different standard for simplifying analysis. For a given operator, off-diagonal elements that are sufficiently small compared to the smallest difference between eigenvalues of the operator can be set equal to zero.

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