Time evolution via a self-consistent maximal-entropy propagation: The reversible case

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A practical approach to the description of time evolution via the mean values of a set of a few relevant observables is discussed. The mean values determine, in a self-consistent way, the time propagation of the system. The procedure yields variational formulation, through which closed-form equations of motion of Hamiltonian form are derived for the relevant mean values. The approximation can provide an exact description under well-defined conditions. The time evolution is reversible in that the entropy does not increase and that it can be described by a unitary evolution operator. A special case of both practical and formal importance is when the relevant observables form a Lie algebra. The self-consistency conditions can then be explicitly implemented and a symplectic structure can be provided for the reduced phase space. Time displacements (of either the state or the observables) can then be described by a self-consistent Hamiltonian, linear in the generators. An example corresponding to the evolution of a Morse-type oscillator under a time-dependent external perturbation is discussed in detail.

I. INTRODUCTION

The use of a few relevant expectation values to characterize the time evolution of small mechanical systems (and, in particular, collisions of composite projectiles[1,2]) is yet without a fully satisfactory theoretical basis. A special case, where an exact description of the evolution is given by such an approach, was previously discussed.[3,4] In that case the Hamiltonian of the system was restricted, however, to be linear in the generators of some Lie algebra. Often, and in many important applications, this is not the case. The subject of this paper is a well-defined approximation which is free from the above limitation. We do, however, restrict the discussion to reversible time evolution (in the sense that the entropy does not change). The more general case of an irreversible evolution is planned to be discussed in a sequel paper.

Our starting point is a requirement of self-consistency on the propagation in time of the relevant observables. This condition and its implications are then rederived using a time-dependent variational principle. Both formulations lead to a close set of equations of motion for the relevant expectation values. These equations of motion can be expressed as Hamilton's equations by the introduction of a set of conjugate variables. The relevant variables are then shown to determine a unique state of maximal entropy[5–7] consistent with the instantaneous values of the observables. The Lagrange multipliers which are so introduced turn out to be the aforementioned conjugate variables. This "Hamiltonian"-like formulation of reversible evolution in terms of relevant expectation values and their conjugate Lagrange multipliers is of interest not only for a reduced description of mechanical systems but also in thermodyamics proper.[8] Determining this Hamiltonian for the propagation of the relevant variables (i.e., imposing self-consistency) requires the explicit construction of a density matrix of maximum entropy at each time step. It is clearly desirable to avoid a repeated solution of such an extremum problem. This is done by assuming that the (if need be, enlarged) set of relevant observables form a Lie algebra. The Hamiltonian of the system, in contrast to the previous formulation, can be any function (not necessarily linear) of the generators. This opens up a wide range of new possible applications. Another bonus is a rich formal geometrical structure which we only briefly explore.

II. THE REDUCED DYNAMICS

Based on physical grounds, the description of deeply inelastic and of transfer collisions in both nuclear[1] and molecular[2] physics is in terms of the time-dependent mean values of a few linearly independent relevant observables. Computational results[9] suggest that such a description is appropriate not only for understanding the final, post-collision state but also during the course of the collision. Similar ideas have been used in the description of the response of a multilevel system to external perturbation.[10] For macroscopic systems[11] such a description has existed for a long time. A particular example is the reversible process of classical thermodyamics.[12]

The most general description of a state in quantum[13] (or classical) mechanics is by a density operator (or function). The state of the system corresponding to the reduced description is thus a density operator parametrized in a unique way by the time-dependent mean values of the (say, $m+1$) linearly independent relevant observables

$$\rho \equiv \rho(\langle A_0 \rangle(t), \ldots, \langle A_m \rangle(t)) \, . \tag{2.1}$$

In (2.1) we have explicitly indicated that the mean values (and hence the state of the system) can vary with time. In what follows we shall not, unless essential, show this dependence explicitly.

An immediate implication of (2.1) is that the time dependence of the density operator is only via the mean values of the relevant observables

$$\partial\rho/\partial t=\sum_{r=0}^{m}(\partial\rho/\partial\langle A_r\rangle)\partial\langle A_r\rangle/\partial t\ . \tag{2.2}$$

The $m+1$ operators $\partial\rho/\partial\langle A_r\rangle$ which appear in (2.2) are biorthogonal to the relevant observables:

$$\mathrm{Tr}(A_s\partial\rho/\partial\langle A_r\rangle)=\partial\mathrm{Tr}(\rho A_s)/\partial\langle A_r\rangle=\delta_s^r\ . \tag{2.3}$$

Here and elsewhere Tr can be understood to stand for integration over a classical phase space, so that the formalism is equally applicable in classical mechanics. In particular, unless otherwise indicated, mean values are over the state ρ given by (2.1), e.g.,

$$\langle A_s\rangle=\mathrm{Tr}(\rho A_s)\ , \tag{2.4}$$

as is consistent with (2.3).

An important special choice of the density operator as a function of the expectation values is the one whose entropy

$$S=-\mathrm{Tr}(\rho\ln\rho) \tag{2.5}$$

is maximal for the given $m+1$ mean values. Then

$$\rho=\exp\left[-\sum_{r=0}^{m}\lambda^r A_r\right]\ . \tag{2.6}$$

The $m+1$ Lagrange multipliers λ^r are functions of the mean values of the relevant observables. They are determined by the condition that at any time t the state (2.6) when used in (2.4) reproduce the $m+1$ mean values at that time t. One can show that this is equivalent to the implicit equation

$$\lambda^r=\partial S/\partial\langle A_r\rangle\ . \tag{2.7}$$

In (2.7) S is the entropy of the state of maximal entropy. An important consequence of (2.7) that we shall often use is the symmetry of the second derivative

$$\partial\lambda^r/\partial\langle A_s\rangle=\partial^2 S/\partial\langle A_r\rangle\partial\langle A_s\rangle=\partial\lambda^s/\partial\langle A_r\rangle\ . \tag{2.8}$$

Using the information theoretic notion of the entropy it is possible to argue[5–7] that the density operator (2.6) provides the "least biased" or "most probable" description of the system. Also, using requirements of consistency it can be shown[14] that the only consistent inference (or induction) for the mean value of some observable B, given the mean values of the relevant observables, is $\mathrm{Tr}(\rho B)$ with ρ given by (2.6). It follows from the Heisenberg equation of motion that the most probable or most consistent estimate for the time rate of change of the relevant mean values is ($B\equiv i[H,A_r]$)

$$\partial\langle A_r\rangle/\partial t=i\,\mathrm{Tr}(\rho[H,A_r])\ . \tag{2.9}$$

In (2.9) the density operator is given by (2.6) with Lagrange multipliers evaluated at the time t.

The equation of motion (2.9) is a trivial consequence of the Heisenberg equation of motion when ρ is an exact solution of the Liouville–von Neumann equation of motion. Otherwise it is by no mean obvious [see (4.8) below] that $\partial\langle A_r\rangle/\partial t\equiv\mathrm{Tr}(A_r\partial\rho/\partial t)$ equals the expectation value of $i[H,A_r]$, computed for ρ at the time t. That the two are equal is our self-consistency condition: propagating the state or propagating the relevant observables should yield identical predictions. Another way of stating the consistency condition is as follows: Given the estimate (2.9) for the "velocities" we have two alternative ways to propagate the density operator. One is to advance the mean values of the relevant observables from the time t to $t+\delta t$. At the new value of the time we use the updated mean values as constraints in the maximum entropy formalism and hence determine updated values of the Lagrange multipliers and the new state. Alternatively, we can propagate the state directly using (2.2). The two alternatives are self consistent in that they can be shown (in Sec. IV) to yield identical results. According to either route the procedure is to start from the relevant mean values to determine the state. Given the state, the mean values can be propagated [using (2.9)]. The new mean values determine the state, and so on.

From now on we shall use the overdot, e.g, as in $\langle\dot{A}_r\rangle$, to mean $\partial\langle A_r\rangle/\partial t\equiv\mathrm{Tr}(A_r\partial\rho/\partial t)$. Only for the relevant observables do we guarantee that $\langle\dot{A}_r\rangle$ is correctly computed by $i\,\mathrm{Tr}(\rho[H,A_r])$. Otherwise we distinguish between the two by the convention introduced above.

The self-consistent scheme as described yields exact results (i.e., equivalent to a solution of the Liouville–von Neumann equation $\dot{\rho}=i[\rho,H]$) whenever there is no error in the estimation of the velocities $\langle i[H,A_r]\rangle$. A sufficient condition[3,4] for the estimate being exact is when the set of relevant observables is closed under commutation with the Hamiltonian:

$$[H,A_r]=\sum_s A_s\alpha^s{}_r\ . \tag{2.10}$$

Here the α's are numerical coefficients. In Sec. III we show that even when (2.10) is not valid, the procedure as outlined provides a variational approximation. In Sec. V we shall construct explicitly a self-consistent Hamiltonian which approximates the actual Hamiltonian H and for which (2.10) is exactly valid.

III. VARIATIONAL PRINCIPLE AND A HAMILTONIAN FORMULATION OF THE REDUCED EQUATIONS OF MOTION

We use a time-dependent variational principle[15,16] which is a natural extension, to density operators and observables, of the Dirac-Frenkel-Schwinger variational principle[17] for wave functions. Just as in the latter the wave function ψ and its dual ψ^* are independent conjugate variables, the observable $A(t)$ and density operator $\rho(t)$ are the independent conjugate variables in the version used here: Defining a Lagrangian $\mathscr{L}$

$$\mathscr{L}=\mathrm{Tr}\{A(t)(\partial\rho/\partial t-i[\rho,H])\}\ , \tag{3.1}$$

the action $\mathscr{S}$,

$$\mathscr{I}=\int_{t_0}^{t_1}\mathscr{L}\,dt-\mathrm{Tr}[\rho(t_1)A(t_1)]\ , \tag{3.2}$$

is made stationary under independent variations $\delta\rho(t)$ and $\delta A(t)$ under mixed boundary conditions[18] $\rho(t_0)=\rho_{\text{in}}$, $A(t_1)=A_{\text{out}}$. The extremum condition $\mathscr{I}=0$ leads to

$$\mathrm{Tr}\{\delta A(t)(\partial\rho/\partial t-i[\rho,H])\}=0\ , \tag{3.3}$$

$$\mathrm{Tr}\{\delta\rho(t)(\partial A/\partial t-i[A,H])\}=0\ . \tag{3.4}$$

When arbitrary variations in $A(t)$ and $\rho(t)$ are allowed, one recovers the exact equations of motion. Here,[19] however, we use a restricted variation in that $\rho(t)$ is parametrized by the mean values of the relevant observables as in (2.1) while $A(t)$ is a linear combination of the relevant observables

$$A(t)=\sum_{r=0}^{m}\lambda^r(t)A_r\ . \tag{3.5}$$

The $m+1$ values $\langle A_r\rangle(t)$ and the $m+1$ time-dependent multipliers $\lambda^r(t)$ are our $2m+2$ variational parameters and are to be varied independently (subject only to the boundary conditions). Of course, ultimately, the multipliers $\lambda^r(t)$ [cf. (3.5)] will turn out to be the Lagrange multipliers of Sec. II. However (and as in the wave-function version of the variational principle), during the variations the mean values and the multipliers are subject to independent variations. In Sec. IV the two independent variations (3.3) and (3.4) will yield the two (equivalent) ways of propagation as discussed in Sec. II.

The variation (3.3) with $A(t)$ parametrized as in (3.5) yields

$$\partial\langle A_r\rangle/\partial t=i\,\mathrm{Tr}(A_r[\rho,H])$$

$$=i\,\mathrm{Tr}(\rho[H,A_r])\ . \tag{3.6}$$

Here ρ is a function of the $m+1$ mean values $\langle A_r\rangle(t)$, cf. (2.1), so that (3.6) implies our estimate (2.8) for the velocities. The nonlinear equations of motion (3.6) are, strictly speaking, independent of the multipliers $\lambda^r(t)$ (since, in principle, ρ is specified by the mean values) and can be solved by themselves. In reality, one must construct ρ in order to evaluate the right-hand side in (3.6). In Sec. V we offer a practical solution for this problem, that is, we shall offer an equation of motion that can be solved without the need for a continuous update of $\rho(t)$. Here we only note that in the special case when (2.10) obtains, the equation of motion becomes linear,

$$\partial\langle A_r\rangle/\partial t=i\sum_s\langle A_s\rangle\alpha^s{}_r\ , \tag{3.7}$$

and it is not necessary to compute expectation values over ρ. The procedure in Sec. V will yield a result similar to (3.7) except that the coefficients α will depend on the mean values.

An equation of motion for the multipliers is obtained from (3.4) using [cf. (2.1)]

$$\delta\rho=\sum_r(\partial\rho/\partial\langle A_r\rangle)\delta\langle A_r\rangle \tag{3.8}$$

and (2.3),

$$\partial\lambda^r/\partial t=\sum_s\lambda^s i\,\mathrm{Tr}\{(\partial\rho/\partial\langle A_r\rangle)[A_s,H]\}\ . \tag{3.9}$$

The equations of motion (3.6) and (3.8) can be cast in the canonical Hamiltonian form

$$\partial\langle A_r\rangle/\partial t=\partial\mathscr{H}/\partial\lambda^r\ , \tag{3.10}$$

$$\partial\lambda^r/\partial t=-\partial\mathscr{H}/\partial\langle A_r\rangle\ , \tag{3.11}$$

where the "Hamiltonian" $\mathscr{H}$ is given by

$$\mathscr{H}=i\sum_r\lambda^r\mathrm{Tr}(\rho[H,A_r])\ . \tag{3.12}$$

The interpretation of these results is provided in Sec. IV.

IV. REDUCED HAMILTONIAN DYNAMICS

The mean values of the relevant observables and their conjugate multipliers can be regarded as a set of generalized coordinates and momenta of a classical phase space.[20] The Poisson bracket[21] in that space is given by

$$\{f,g\}=\sum_r[(\partial f/\partial\langle A_r\rangle)(\partial g/\partial\lambda^r)$$

$$-(\partial f/\partial\lambda^r)(\partial g/\partial\langle A_r\rangle)]\ . \tag{4.1}$$

The Hamiltonian $\mathscr{H}$ as defined in (3.12) is the generator of the time displacement not only for the conjugate canonical coordinates

$$\{\langle A_r\rangle,\lambda^s\}=\delta_r{}^s\ , \tag{4.2}$$

$$\{\mathscr{H},\langle A_r\rangle\}=\langle\dot{A}_r\rangle\ , \tag{4.3}$$

$$\{\mathscr{H},\lambda^s\}=\dot{\lambda}^s \tag{4.4}$$

but also for any other observable

$$\{\mathscr{H},\langle B\rangle\}=\langle\dot{B}\rangle\ . \tag{4.5}$$

Here, as elsewhere, expectation values are over ρ and the proof of (4.5) is using (2.2) and (3.10). The overdot denotes a time derivative. The purpose of this section is to note the main characteristics of the motion in this phase space with special reference to its reversible character.

A. Entropy and other invariants

There are many density operators consistent with the given mean values of the relevant observables, with different values of the entropy, $-\mathrm{Tr}(\rho\ln\rho)$. The reduced description is here defined by choosing the one density operator whose entropy is maximal. We thereby have a description in a $(2m+2)$-dimensional reduced phase space. In that reduced space, the entropy corresponding to given $m+1$ values of the relevant observables is unique. As is only to be expected for a (classical) Hamiltonian ($\mathscr{H}$) motion—this entropy does not change with time. The formal proof uses the conservation of normalization ($d\langle 1\rangle/dt=0$) and Eqs. (2.2), (2.6), and (3.6) to conclude that

$$dS/dt=-\mathrm{Tr}(\dot{\rho}\ln\rho)=-\sum_r \mathrm{Tr}[(\partial\rho/\partial\langle A_r\rangle)\ln\rho]\langle \dot{A}_r\rangle$$
$$=\sum_{r,s}\lambda^s \mathrm{Tr}[(\partial\rho/\partial\langle A_r\rangle)A_s]\langle \dot{A}_r\rangle=\sum_s \lambda^s\langle \dot{A}_s\rangle$$
$$=i\sum_s \lambda^s \mathrm{Tr}(\rho[H,A_s])=-i\,\mathrm{Tr}(\rho[H,\ln\rho])$$
$$=i\,\mathrm{Tr}(H[\rho,\ln\rho])=0\ . \tag{4.6}$$

Note that in (4.6) the λ^r's are the Lagrange multipliers of (2.6) and that we will shortly show their equivalence to the multipliers of Sec. III.

The proof of the invariance of the entropy uses in an essential way the linearity of $\ln\rho$ in the relevant observables. Indeed, in general, only when an observable C is a linear combination of the relevant observables will it be the case that

$$d\langle C\rangle/dt\equiv\mathrm{Tr}(\dot{\rho}C)=i\,\mathrm{Tr}(\rho[H,C])\ . \tag{4.7}$$

The proof is immediate. In general

$$\partial\langle C\rangle/dt=\sum_r \mathrm{Tr}[(\partial\rho/\partial\langle A_r\rangle C)]\langle \dot{A}_r\rangle$$
$$=i\sum_r \mathrm{Tr}[(\partial\rho/\partial\langle A_r\rangle)C]\mathrm{Tr}(\rho[H,A_r])\ .$$

If, however, $C=\sum_s \gamma^s A_s$ then the orthogonality condition (2.3) comes into play so that

$$\partial\langle C\rangle/dt=\sum_s \gamma^s i\,\mathrm{Tr}(\rho[H,A_s])=i\,\mathrm{Tr}(\rho[H,C])\ . \tag{4.8}$$

It should now be obvious that the self-consistency condition (2.6) is nontrivial. It need not hold for observables not in the space of relevant ones. In particular, a strict constant of the motion D, defined by $[D,H]=0$, may, in the reduced classical phase space, correspond to an expectation value $\langle D\rangle=\mathrm{Tr}(\rho D)$ which will vary with time. The reason is obvious. $\langle D\rangle$ is our "best" estimate and our estimate may not be good enough. The constants of motion in the classical phase space are those functions which satisfy

$$\{\phi,\mathscr{H}\}=0\ . \tag{4.9}$$

The entropy $S=\sum_r \lambda^r\langle A_r\rangle$ is one such function. In Sec. IV C we shall explicitly identify m additional ones. Indeed, we shall conclude that the equations of motion (4.3) and (4.4) are completely integrable.[22]

B. The Lagrange multipliers and self-consistency

The conservation of entropy offers a simple route to the identification of the Lagrange multipliers as the variables that satisfy the equation of motion (3.9). Throughout the proof below the λ^r's are the Lagrange multipliers determined via the procedure of maximum entropy. Hence they can be considered as functions of the relevant expectation values

$$\dot{\lambda}^r=\sum_s(\partial\lambda^r/\partial\langle A_s\rangle)\langle \dot{A}_s\rangle \tag{4.10}$$

or, using the symmetry relation (2.8),

$$\dot{\lambda}^r=\sum_s(\partial\lambda^s/\partial\langle A_r\rangle)\langle \dot{A}_s\rangle\ .$$

It follows that

$$\dot{\lambda}^r+\sum_s\lambda^s(\partial\langle \dot{A}_s\rangle/\partial\langle A_r\rangle)=\partial\left[\sum_s\lambda^s\langle \dot{A}_s\rangle\right]\Big/\partial\langle A_r\rangle\ . \tag{4.11}$$

It is important to note that on the right-hand side of (4.11) $\sum\lambda^s\langle \dot{A}_s\rangle$ is only a function of the mean values of the relevant observables. Indeed, it equals [cf. (4.6)] $i\,\mathrm{Tr}(H[\rho,\ln\rho])$ and hence vanishes for any set of mean values. Therefore its derivative vanishes as well. In a reversible process it thus follows that

$$\dot{\lambda}^r=-\sum_s\lambda^s(\partial\langle \dot{A}_s\rangle/\partial\langle A_r\rangle)$$
$$=-i\sum_s\lambda^s\mathrm{Tr}\{[H,A_s](\partial\rho/\partial\langle A_r\rangle)\}\ . \tag{4.12}$$

Comparing with (3.9), the Lagrange parameters satisfy the same first-order equation of motion as the variational parameters of Sec. III. It follows that one can identify $A(t)$,

$$A(t)=\sum_r\lambda^r(t)A_r \tag{3.5'}$$

with the surprisal[4,19,23] $(-\ln\rho)$.

The self-consistent reversible propagation can thus be schematically illustrated as (where ME denotes maximal entropy)

$$\begin{array}{ccc}\langle A_r\rangle(t) & \xrightarrow{\partial\mathscr{H}/\partial\lambda^r} & \langle A_r\rangle(t+\delta t)\\ \Big\downarrow \mathrm{ME} & & \Big\downarrow \mathrm{ME}\\ \rho(t) & \xrightarrow[-\partial\mathscr{H}/\partial\langle A_r\rangle]{} & \rho(t+\delta t)\ .\end{array} \tag{4.13}$$

What (4.12) and (3.9) show is that the two sides of the diagram commute. Starting with the mean values of the relevant observables at the time t one obtains the same $\rho(t+\delta t)$ whether one first propagates the mean values to the time $t+\delta t$ [using the variation (3.3) or the explicit result (3.6)] and then the procedure of maximal entropy or whether one first uses maximal entropy to determine the Lagrange multipliers at the time t and then propagate them [using the variation (3.4) or the explicit result (3.9)] to $t+\delta t$. In other words, the reversible time evolution commutes with projecting onto the state of maximal entropy.

C. Complete integrability

The identification of the variational parameters $\{\lambda^r(t)\}$ with the Lagrange multipliers provides also the proof that the Hamiltonian system (4.2)–(4.5) is completely integrable.[22] In other words, it has $m+1$ linearly independent constants of the motion

$$\{\mathscr{H},\phi_r\}=0 \tag{4.14}$$

which are in involution

$$\{\phi_r,\phi_s\}=0\ . \tag{4.15}$$

The motion in the $(2m+2)$-dimensional phase space is thus restricted to an $(m+1)$-dimensional manifold. (In Sec. V we shall derive the equations of motion on this manifold.)

We shall prove the results for the choice (where $A_0=I$)

$$\phi_r(\vec{\lambda},\langle\vec{A}\rangle)=\langle A_r\rangle-\mathrm{Tr}\left[A_r\exp\left[\lambda_0-\sum_s\lambda^s A_s\right]\right] . \quad (4.16)$$

Now

$$\partial\phi_r/\partial\langle A_v\rangle=\delta_r{}^v \quad (4.17)$$

and because of the symmetry (2.8)

$$\partial\phi_r/\partial\lambda^s=\partial\phi_s/\partial\lambda^r . \quad (4.18)$$

Using the definition (4.1) of the Poisson bracket, (4.17), and (4.18), one verifies (4.15). Also

$$\dot{\phi}_r=\{\mathscr{H},\phi_r\}=\sum_s[(\partial\mathscr{H}/\partial\langle A_s\rangle)(\partial\phi_r/\partial\lambda^s)-(\partial\phi_r/\partial\langle A_s\rangle)(\partial\mathscr{H}/\partial\lambda^s)]$$

$$=-\sum_s\dot{\lambda}^s(\partial\phi_r/\partial\lambda^s)-\langle\dot{A}_r\rangle=0 . \quad (4.19)$$

The last expression equals zero because of (4.10) since

$$\sum_s(\partial\phi_r/\partial\lambda^s)(\partial\lambda^s/\partial\langle A_v\rangle)=\delta_r{}^v . \quad (4.20)$$

V. LIE ALGEBRA OF RELEVANT OBSERVABLES

There are several motivations for introducing the special case where the relevant observables are generators of a Lie group (that is, they form a Lie algebra). The more pragmatic one is that constructing a state of maximal entropy is far simpler than for the general case of noncommuting observables. Indeed, it is so simple that we shall be able to derive explicit equations of motion. Next, as will be discussed in detail below, such a set of observables is ideally suited for reversible (constant entropy) motion. The result is that we can take full advantage of the complete integrability and work with $m+1$ (or less) equations of motion rather than with the $2(m+1)$ equations of the general case. Finally, and as will be discussed in detail in Sec. V G the number of generators that need to be included can be smaller than the number of relevant observables. On the formal level, the formalism is a natural generalization of the coherent-state representation[17,20,24] which was employed in the Dirac-Frenkel variational principle. It thus admits of a symplectic manifold structure on the $(m+1)$-dimensional reduced space [as opposed to the $2(m+1)$-dimensional space in the general (not necessarily reversible) case]. As will also be shown, it is often possible to restrict the motion to an even-dimensional submanifold of the $(m+1)$-dimensional manifold. In the following sections we restrict the discussion to semisimple Lie groups.

A. Parametrization of the state

A set of states of equal entropy can be generated by the unitary transformation[25]

$$U(\vec{\xi})=\exp(i\xi^\mu X_\mu) . \quad (5.1)$$

Here $U(\xi)$ is an element of a Lie group. The generators $\{X_\mu\}$ of the group form a Lie algebra

$$[X_\mu,X_\nu]=C^\lambda{}_{\mu\nu}X_\lambda . \quad (5.2)$$

The C's are structure constants of the algebra. Given an initial state ρ_0 the states at other times are given by

$$\rho(\xi)=U(\xi)\rho_0U^\dagger(\xi) . \quad (5.3)$$

The group parameters $\{\xi^\mu\}$ are regarded as functions of time and the purpose of this section is to determine their equation of motion and its properties.

The parametrization (5.3) clearly preserves the normalization and entropy for any set of (real) group parameters ξ. Furthermore, if ρ_0 is of maximal entropy subject to the mean values of the relevant observables, the group generators,

$$\rho_0=\exp(-\lambda^0{}_0-\lambda^r{}_0X_r) , \quad (5.4)$$

then so is any other $\rho(\xi)$

$$\rho(\xi)=\exp[-\lambda^0(\xi)-\lambda^r(\xi)X_r] . \quad (5.5)$$

The proof follows immediately from the automorphism of the Lie algebra by the corresponding group:

$$U(\xi)X_rU^\dagger(\xi)=G^s{}_r(\xi)X_s . \quad (5.6)$$

The elements of the G matrix[3] in (5.6) will of course depend on the value of ξ. Now

$$\rho(\xi)=U\rho_0U^\dagger=\exp(-\lambda^0{}_0-\lambda^r{}_0UX_rU^\dagger) . \quad (5.7)$$

Hence, using (5.6) and comparing (5.7) and (5.5),

$$\lambda^s(\xi)=\lambda^r{}_0G^s{}_r(\xi) . \quad (5.8)$$

In Sec. V G we prove a generalization of (5.5) where ρ_0 is of maximal entropy subject to additional constraints.

B. The product representation

For practical work the product (global) representation[26]

$$U(\vec{\eta})=\prod_\lambda\exp(i\eta^\lambda X_\lambda) \quad (5.9)$$

of the elements of the Lie group is more convenient. The reason is that it is frequently necessary to differentiate ρ with respect to the group parameters. Now, for either (5.1) or (5.9) one has a similar form for the result:[3,27]

$$\partial U/\partial\xi^\mu=i\hat{X}_\mu U , \quad (5.10)$$

$$\partial U/\partial\eta^\mu=i\hat{X}_\mu U . \quad (5.11)$$

$\hat{X}_\mu$ is a linear combination of the generators (see Appendix A)

$$\hat{X}_\mu=D^\nu{}_\mu X_\nu , \quad (5.12)$$

where the matrix D is nonsingular. The matrix D is different for (5.10) and (5.11) but is much more readily computed as a function of the group parameters for the product representation,[26] where all one requires is the matrix

G defined by the automorphism (5.6). The explict construction, for both representations, is given in Appendix A.

In the formal discussion one need not commit oneself to a particular representation for U, hence $\hat{X}_\mu$ can stand for the result of either (5.10) or (5.11). Also, we shall use η for the group parameters but in this section η can also be understood as ξ. This will of course no longer be the case in the example discussed in Sec. VI.

The dependence of ρ on the group parameters can now be determined:

$$\partial\rho/\partial\eta^\lambda=(\partial U/\partial\eta^\lambda)\rho_0 U^\dagger+U\rho_0(\partial U^\dagger/\partial\eta^\lambda)$$
$$=i\hat{X}_\lambda\rho-i\rho\hat{X}_\lambda=i[\hat{X}_\lambda,\rho]\ . \tag{5.13}$$

Then for any observable B

$$\partial\langle B\rangle/\partial\eta^\lambda=\mathrm{Tr}(B\partial\rho/\partial\eta^\lambda)=i\ \mathrm{Tr}(B[\hat{X}_\lambda,B])\ .$$
$$=-i\ \mathrm{Tr}(\rho[\hat{X}_\lambda,B])\ . \tag{5.14}$$

In particular, for the mean values of the relevant observables

$$\partial\langle X_\nu\rangle/\partial\eta^\mu=-i\ \mathrm{Tr}(\rho[\hat{X}_\mu,X_\nu]) \tag{5.15}$$

or, using the matrix D [cf. (5.12)], one can introduce an antisymmetric matrix σ:

$$\sigma_{\mu\lambda}=(\partial\langle X_\mu\rangle/\partial\eta^\nu)D_\lambda{}^\nu=-i\ \mathrm{Tr}(\rho[\hat{X}_\mu,\hat{X}_\lambda])\ . \tag{5.16}$$

This matrix will play a key role in the formal considerations of Sec. V C coming up. The discussion of the dynamics begins in Sec. V D and one can proceed directly to that section.

C. The symplectic structure

In Secs. II–IV we have considered the general case where the Lagrange multipliers and their conjugate relevant mean values are considered as $2(m+1)$ independent generalized coordinates. For the reversible case the motion was shown to be confined to a lower-dimensional manifold. In this section we discuss the motion on that manifold alone and show that it too can be considered as a phase space of dimension $m+1$ at most.

For the parametrization (5.3) the expectation value of any observable F is a function of the group parameters

$$F(\eta)\equiv\mathrm{Tr}[F\rho(\eta)]\ . \tag{5.17}$$

We note again that here and throughout Sec. V η can just as well be ξ. If the antisymmetric matrix σ, (5.16), can be inverted

$$\sigma^{\mu\nu}\sigma_{\nu\lambda}=\delta^\mu{}_\lambda \tag{5.18}$$

one can define a generalized Poisson bracket[21] for any two expectation values, which are the "classical" dynamial variables in the reduced description

$$\{F(\eta),G(\eta)\}\equiv\frac{\partial F}{\partial\eta^\mu}\sigma^{\mu\nu}\frac{\partial G}{\partial\eta^\nu}\ . \tag{5.19}$$

It is readily verified that this definition satisfies the requirements, is an antisymmetric bilinear product in F and G, and that it satisifes the Jacobi identity.[28] The proof of the identity is based on noting that

$$\partial\sigma_{\alpha\beta}/\partial\eta^\gamma=\mathrm{Tr}(\rho[[\hat{X}_\alpha,\hat{X}_\beta],\hat{X}_\gamma]) \tag{5.20}$$

and that

$$\{\{F,G\},K\}+\{\{G,K\},F\}+\{\{K,F\},G\}$$
$$=F^\alpha G^\beta K^\gamma(\partial\sigma_{\beta\gamma}/\partial\eta^\alpha+\partial\sigma_{\gamma\alpha}/\partial\eta^\beta+\partial\sigma_{\alpha\beta}/\partial\eta^\gamma)\ , \tag{5.21}$$

where

$$F^\alpha=\sigma^{\alpha\beta}\partial F(\eta)/\partial\eta^\beta\ . \tag{5.22}$$

Inserting (5.20) into (5.21) we see that (5.21) must be 0, so that the Jacobi identity for the Poisson brackets (5.19) is implied by the Jacobi identity for the operators of the algebra. The whole question then is whether σ is invertible.

We have another motivation for requiring that $\sigma_{\mu\nu}$ is invertible. A classical phase space is required to admit canonical coordinate charts. An arbitrary chart $(\eta^1,\eta^2,\ldots)$ in a neighborhood is said[29] to be "locally canonical" if the matrix

$$\sigma^{\mu\nu}=\{\eta^\nu,\eta^\mu\} \tag{5.23}$$

is nonsingular and can be brought to the canonical form

$$\{\sigma^{\mu\nu}\}\equiv\begin{bmatrix}\underline{0} & -\underline{I}\\ \underline{I} & \underline{0}\end{bmatrix} \tag{5.24}$$

at each point of the neighborhood. A necessary and sufficient condition for the existence of local coordinate charts is[29] that the matrix defined by (5.23) is invertible. But with the definition (5.19), that is the same as the condition that the matrix $\sigma_{\mu\nu}$ as defined by (5.18) and (5.16) is invertible. If σ is indeed invertible, the properties of the reduced phase space are those of a symplectic manifold.[29,30] That σ is invertible is not automatically guaranteed since, for example, the dimension of the algebra may just as well be odd and the phase space must be even-dimensional. However, for the case of quotient space in semisimple Lie groups this inversion is assured.[31]

The stability group H of the reference state ρ_0 [cf. (5.3)] is defined[17,31] as the set of all elements $h\in G$ (where G is the full Lie group) that leave ρ_0 invariant,

$$h\rho_0 h^{-1}=\rho_0\ . \tag{5.25}$$

For any $g\in G$ it follows that

$$\rho(g)=g\rho_0 g^{-1}=gh\rho_0 h^{-1}g^{-1}\ , \tag{5.26}$$

where $h\in H\subset G$ and H is the stability group of ρ_0. The only transformations of ρ_0 which serve to change the state are thus those induced by the quotient space G/H. In other words, the set of orbits[17,32] of the state ρ_0 by the Lie group G,

$$M=\{\rho(\eta)\,|\,\rho(\eta)=g(\eta)\rho_0 g^{-1}(\eta),\ g\in G\}\ , \tag{5.27}$$

is realized by the homogeneous space G/H. Any element

gH in the quotient space G/H can be represented as

$$gH=\exp(X)H\ , \tag{5.28}$$

where X is in the complement vector space $\tilde{k}$ of the stability group H:

$$\tilde{g}=\tilde{h}\oplus\tilde{k}\ , \tag{5.29}$$

where $\tilde{g}$ and $\tilde{h}$ are the Lie algebras of G and H, respectively.

To conclude, it is sufficient to consider the group elements

$$U(\eta)=\prod_{\mu}\exp(i\eta^{\mu}X_{\mu})$$

or (5.30)

$$U(\xi)=\exp(i\xi^{\mu}X_{\mu})\ ,$$

where $\{X_{\mu}\}$ is a basis for $\tilde{k}$, without any loss of generality. The group parameters need be independent parameters only in G/H. The manifold M may or may not be symplectic. If the full Lie group is of odd dimensions (as is the case for example of Sec. VI) but so is the stability group, then the quotient space will be even-dimensional and the manifold will be symplectic. In the following we will assume that ρ_0 has been chosen such that M is even-dimensional so that $\sigma_{\mu\nu}$ can be nonsingular. The equations of motion below will thus be for the parameters of the quotient space G/H.

D. Hamiltonian dynamics on a symplectic manifold

We derive Hamiltonian equations of motion for the group parameters and for any dynamical variable $F(\eta)=\mathrm{Tr}[F\rho(\eta)]$. The role of the Hamiltonian will thus be played by $H(\eta)$,

$$H(\eta)=\mathrm{Tr}[H\rho(\eta)] \tag{5.31}$$

and the Poisson brackets are defined by (5.19).

The construction begins with the Lagrangian $\mathscr{L}$, (3.1), which is here a function of η's [via $\rho(\eta)$] and of λ's [via $A(t)$, cf. (3.5)]:

$$\begin{aligned}\mathscr{L}&=\mathrm{Tr}[A(t)\dot{\rho}]-i\,\mathrm{Tr}\{A(t)[\rho,H]\}\\&=\lambda^{\nu}\mathrm{Tr}[X_{\nu}(\partial\rho/\partial\eta^{\mu})]\dot{\eta}^{\mu}-\lambda^{\nu}i\,\mathrm{Tr}\{\rho(\eta)[H,X^{\nu}]\}\ .\end{aligned} \tag{5.32}$$

Using (5.14) and (5.12),

$$\mathscr{L}=\lambda^{\nu}(\partial\langle X_{\nu}\rangle/\partial\eta^{\mu})\dot{\eta}^{\mu}-\lambda^{\mu}(D^{-1})_{\mu}[\partial H(\eta)/\partial\eta^{\nu}]\ .$$

With the use of the definition (5.16), the first Euler-Lagrange equation is given by

$$\sigma_{\nu\mu}\dot{\eta}^{\mu}=\partial H(\eta)/\partial\eta^{\nu}\ . \tag{5.33}$$

Under our choice of ρ_0 which insures that σ is invertible this can be written in a canonical Hamiltonian form [cf. (5.24)]

$$\dot{\eta}^{\mu}=\sigma^{\mu\nu}\partial H(\eta)/\partial\eta^{\nu}\ . \tag{5.34}$$

It is worthwhile to emphasize that the group parameters provide a complete set of coordinates for our phase space. This is particularly obvious when the antisymmetric matrix σ is brought to the canonical form (5.24).

The second Euler-Lagrange equation is for the $\dot{\lambda}$'s. It is equivalent to (3.9) and provides no new information beyond (5.34). This is as it should be since we have introduced the parametrization $\rho(\eta)$ to take full advantage of the fact that for reversible motion the Lagrange multipliers are completely determined by the mean values of the relevant observables. Indeed, we could have used the mean values of the observables [which need be only those in the quotient space, cf. (5.28)] as the coordinates of the phase space. To do so we write [cf. (5.15)]

$$\langle\dot{X}_{\nu}\rangle=(\partial\langle X_{\nu}\rangle/\partial\eta^{\mu})\dot{\eta}^{\mu}$$

and, using (5.16) and (5.34),

$$\begin{aligned}\langle\dot{X}_{\nu}\rangle&=(\partial\langle X_{\nu}\rangle/\partial\eta^{\mu})\sigma^{\mu\lambda}\partial H/\partial\eta^{\lambda}\\&=\partial H(\eta)/\partial\hat{\eta}^{\nu}=\sigma_{\nu\mu}\partial H(\eta)/\partial\langle X_{\mu}\rangle\ .\end{aligned} \tag{5.35}$$

In (5.35) we have introduced $\hat{\eta}^{\nu}$ as the contragradient transformation to (5.12). In other words, we write (5.13) as

$$\partial\rho/\partial\hat{\eta}^{\nu}=i[X_{\nu},\rho]\ . \tag{5.36}$$

In terms of the $\hat{\eta}$'s the Hamiltonian $H(\eta)$ can be written as

$$H(\eta)=\lambda^{\nu}\partial\mathscr{H}/\partial\hat{\eta}^{\nu} \tag{5.37}$$

from which the result (3.10) is seen to be equivalent to (5.32). As a consistency check we also verify from (5.35) and (5.36) that

$$\langle\dot{X}_{\nu}\rangle=i\,\mathrm{Tr}\{\rho(\eta)[H,X_{\nu}]\} \tag{5.38}$$

as should be the case for self-consistency.

Using the Poisson brackets defined by (5.19) we can now write a Hamiltonian equation of motion for any dynamical variable $B(\eta)\equiv\mathrm{Tr}[B\rho(\eta)]$,

$$\dot{B}(\eta)=\{H(\eta),B(\eta)\}\ . \tag{5.39}$$

The equation is analogous but not identical to (4.5). In (5.39) $H(\eta)$ [and $B(\eta)$] are only functions of the group parameters (or, alternatively, of the mean values of the relevant observables) and these are fewer in number.

Finally, we note that our original objective has been achieved. The equations of motion (5.34) can be solved directly without the need to update the maximum entropy estimate of ρ after each time step. What replaces the updating of the state is the updating of the observables via the automorphism (5.6). But the G matrix can be computed once as a function of the group parameters and then used throughout the computation. (An example is provided in Sec. VI.) In general, updating the state and updating the observables need not yield the same results (apart from, say, in an exact computation). The parametrization (5.3) insures however that the two routes are equivalent.

E. The linear self-consistent Hamiltonian

The discussion in Sec. V D has been in terms of classical dynamical variables which are expectation values of

operators. Here we provide the corresponding formalism directly in terms of operators. Central to the discussion is the self-consistent Hamiltonian operator $\mathcal{H}$, defined by

$$\mathcal{H}=\sigma^{\mu\nu}[\partial H(\eta)/\partial\eta^{\mu}]\hat{X}_{\nu}=i\sigma^{\mu\nu}\mathrm{Tr}(\rho[H,\hat{X}_{\mu}])\hat{X}_{\nu} , \tag{5.40}$$

which is linear in the generators of the group.

The self-consistent Hamiltonian attains its special position since it acts as the true Hamiltonian as far as the operators of the algebra are concerned. We prove this in two ways. First in obtaining a Liouville-von Neumann equation of motion for the density operator:

$$\begin{aligned}\dot{\rho}&=(\partial\rho/\partial\eta^{\mu})\dot{\eta}^{\mu}\\&=(\partial\rho/\partial\eta^{\mu})\sigma^{\mu\nu}[\partial H(\eta)/\partial\eta^{\nu}]=\{\rho,H\}\\&=i[\rho,\hat{X}_{\mu}]\sigma^{\mu\nu}[\partial H(\eta)/\partial\eta^{\nu}]\end{aligned} \tag{5.41}$$

or, from the definition (5.40) of $\mathcal{H}$,

$$\dot{\rho}=i[\mathcal{H},\rho] . \tag{5.42}$$

This equation of motion is nonlinear in ρ (since the self-consistent Hamiltonian $\mathcal{H}$ depends on the state) yet it preserves the entropy of ρ.

The corresponding result for observables is that for any operator A,

$$A=\hat{c}^{\alpha}X_{\alpha}=c^{\alpha}\hat{X}_{\alpha} \tag{5.43}$$

which is a linear combination of operators in the algebra

$$\mathrm{Tr}(\rho[H,A])=\mathrm{Tr}(\rho[\mathcal{H},A]) . \tag{5.44}$$

The proof uses the definitions of A and of $\mathcal{H}$ [Eq. (5.40)], of $\hat{X}$ [Eq. (5.12)], and of σ [Eqs. (5.15)—(5.18)] as follows:

$$\begin{aligned}\mathrm{Tr}(\rho[\mathcal{H},A])&=c^{\alpha}\mathrm{Tr}(\rho[\mathcal{H},\hat{X}_{\alpha}])\\&=\sigma^{\mu\nu}\mathrm{Tr}(\rho[H,\hat{X}_{\mu}])c^{\alpha}\mathrm{Tr}(\rho[\hat{X}_{\nu},\hat{X}_{\alpha}])\\&=\sigma^{\mu\nu}\sigma_{\nu\alpha}c^{\alpha}\mathrm{Tr}(\rho[H,\hat{X}_{\mu}])\\&=c^{\alpha}\mathrm{Tr}(\rho[H,\hat{X}_{\alpha}])=\mathrm{Tr}(\rho[H,A]) .\end{aligned} \tag{5.45}$$

Another point of view of $\mathcal{H}$ is as the "relevant part"[32] of the full Hamiltonian H. For an arbitrary operator F one defines the relevant part as that operator whose expectation value will be correctly predicted given only the mean values of the relevant observables. It is convenient to introduce[11] a (projection) operator P such that PF,

$$\begin{aligned}PF&\equiv\mathrm{Tr}[(\partial\rho/\partial\langle\hat{X}_{\mu}\rangle)F]\hat{X}_{\mu}\\&=(\partial\eta^{\nu}/\partial\langle\hat{X}_{\mu}\rangle)\mathrm{Tr}[(\partial\rho/\partial\eta^{\nu})F]\hat{X}_{\mu}\\&=i\sigma^{\nu\mu}\mathrm{Tr}(\rho[\hat{X}_{\nu},F]\hat{X}_{\mu} ,\end{aligned} \tag{5.46}$$

is the relevant part of F. Using (5.12)—(5.18),

$$P\hat{X}_{\mu}=\hat{X}_{\mu} \tag{5.47}$$

so that P is a projection and from the definition of $\mathcal{H}$,

$$\mathcal{H}=PH . \tag{5.48}$$

The "residual" interaction

$$V\equiv H-\mathcal{H}$$

is either nonlinear in the generators of G or zero. The nature of the reversible approximation of this paper is to neglect the role of V. A higher-order irreversible reduced description will be discussed in a sequel paper.

F. The quality of the variational approximation

It was already pointed out[3] that the approach of this paper will give exact results whenever the set of relevant observables is closed under commutation with the true Hamiltonian H,

$$[H,X_{\mu}]=X_{\nu}\alpha^{\nu}{}_{\mu} . \tag{2.10'}$$

The nature of the variational approximation can thus be stated that we satisfy the relevant part of (2.10'):

$$[\mathcal{H},X_{\mu}]=X_{\nu}\alpha^{\nu}{}_{\mu} . \tag{5.49}$$

Here, however, the coefficients α do depend on the state

$$\alpha^{\nu}{}_{\mu}=\mathrm{Tr}\{(\partial\rho(\eta)/\partial\langle X_{\nu}\rangle)[H,X_{\mu}]\} , \tag{5.50}$$

where (5.50) follows directly from the variational equation of motion (3.9). It is thus possible to rewrite (3.9) as

$$\partial\lambda^{\nu}/\partial t=-\alpha^{\nu}{}_{\mu}\lambda^{\mu} , \tag{5.51}$$

where the point is that $\alpha^{\nu}{}_{\mu}$ can be regarded as a function of the time only. The reason being that the equations of motion for the expectation values $\langle X_{\nu}\rangle$ or for the group parameters η^{μ} can be solved without reference to the Lagrange multipliers. [This is also true in the $(2m+2)$-dimensional reduced space of Secs. III and IV.] The solution [of (5.34) or of (5.35)] can be used in (5.50) so that in (5.51) α can be regarded as a function of time only. The integrated version of (5.51) is

$$\lambda^{\nu}(t)=\exp\left[-\int_{t_0}^{t}\alpha^{\nu}{}_{\mu}(t')dt'\right]\lambda^{\mu}{}_{0} . \tag{5.52}$$

This identifies the $G(\eta)$ matrix of (5.8) with the integral in (5.52) just as in the exact approach.[3]

Approximate (in the sense of the variational approximation) time-dependent constants of the motion[33] can therefore be introduced. For example, since for any reference state $-\ln\rho=\lambda^{\mu}X_{\mu}$ is a constant of the motion, we have that [cf. (5.8)]

$$\begin{aligned}\lambda^{\mu}(t)\langle X_{\mu}\rangle(t)&=\lambda^{\nu}{}_{0}\langle X_{\nu}\rangle(t_0)\\&=\lambda^{\nu}{}_{0}G^{\mu}{}_{\nu}\langle X_{\mu}\rangle(t) .\end{aligned} \tag{5.53}$$

Equation (5.53) holds for any choice of the $\lambda^{\nu}{}_{0}$'s so that

$$\langle X_{\mu}\rangle(t)=F^{\nu}{}_{\mu}\langle X_{\nu}\rangle(t_0) , \tag{5.54}$$

where F is the inverse of the G matrix.

The linear transformation between the precollision and post-collision expectation values of the relevant observables is known as a "sum rule." Such relations are often known on phenomenological grounds (see, e.g., their use in Ref. 34). Also, they often emerge as the final result of physically motivated simple models. Whenever such sum rules are known to be more or less valid or useful the vari-

ational approximation using the respective operators as relevant observables will be reasonable.

G. The reference state

It might appear that the formalism introduced in this section allows for only a very limited choice of reference states ρ_0 [cf. (5.3)], namely, those given by (5.4). It is therefore important to dispel any such misconceptions by showing explicitly that at the very least all reference states of the generic form

$$\rho_0=\exp(-\lambda_0-\lambda^{\mu}{}_0X_{\mu}-\lambda^{\mu\nu}{}_0X_{\mu}X_{\nu}-\cdots) \tag{5.55}$$

are equally admissible. An example is provided in Sec. VI.

States of the form (5.55) are of maximal entropy subject to the mean values of polynomials in the operators of the algebra. (The set of all such polynomials is known as the enveloping field of the algebra.[35,31])

The proof starts from the automorphism of the algebra proper,

$$U(\eta)X_{\nu}U^{\dagger}(\eta)=G^{\mu}{}_{\nu}(\eta)X_{\mu} \tag{5.6'}$$

so that

$$UX_{\alpha}X_{\beta}U^{\dagger}=UX_{\alpha}U^{\dagger}UX_{\beta}U^{\dagger}=G^{\nu}{}_{\alpha}G^{\mu}{}_{\beta}X_{\nu}X_{\mu}\ . \tag{5.56}$$

An nth power of the generators transforms therefore as a tensor of rank n

$$UX_{\alpha_1}\cdots X_{\alpha_n}U^{\dagger}=G^{\mu_1}{}_{\alpha_1}\cdots G^{\mu_n}{}_{\alpha_n}X_{\mu_1}\cdots X_{\mu_n}\ . \tag{5.57}$$

Also, the nth powers are closed under commutation with the generators

$$\begin{aligned}&[X_{\nu},X_{\mu_1},\ldots,X_{\mu_n}]\\&\quad=[X_{\nu},X_{\mu_1}]X_{\mu_2}\cdots X_{\mu_n}+\cdots\\&\qquad+X_{\mu_1}\cdots X_{\mu_{n-1}}[X_{\nu},X_{\mu_n}]\\&\quad=C^{\mu}{}_{\nu\mu_1}X_{\mu}X_{\mu_2}\cdots X_{\mu_n}+\cdots\\&\qquad+C^{\mu}{}_{\nu\mu_n}X_{\mu_1}\cdots X_{\mu_{n-1}}X_{\mu_n}\ .\end{aligned} \tag{5.58}$$

It follows that if ρ_0 is of the generic form (5.55) so is ρ and the highest power of the generators that appears in ρ_0 is also the highest power in ρ:

$$\begin{aligned}\rho&=U\rho_0U^{\dagger}=\exp(-\lambda_0-\lambda^{\mu}{}_0UXU^{\dagger}-\lambda^{\mu\nu}{}_0UX_{\mu}X_{\nu}U^{\dagger}-\cdots)\\&=\exp(-\lambda_0-\lambda^{\mu}{}_0G^{\alpha}{}_{\mu}X_{\alpha}-\lambda^{\mu\nu}{}_0G^{\alpha}{}_{\mu}G^{\beta}{}_{\nu}X_{\alpha}X_{\beta}-\cdots)\\&=\exp(-\lambda_0-\lambda^{\alpha}X_{\alpha}-\lambda^{\alpha\beta}X_{\alpha}X_{\beta}-\cdots)\ .\end{aligned} \tag{5.59}$$

The Lagrange parameters are propagated in a contragradient manner to the observables

$$\begin{aligned}\lambda^{\alpha}&=\lambda^{\mu}{}_0G^{\alpha}{}_{\mu}\ ,\\\lambda^{\alpha\beta}&=\lambda^{\mu\nu}{}_0G^{\alpha}{}_{\mu}G^{\beta}{}_{\nu}\ ,\end{aligned} \tag{5.60}$$

etc.

The entropy of ρ can also be resolved according to the power of the generators which act as the constraints:

$$\begin{aligned}S&\equiv-\mathrm{Tr}(\rho\ln\rho)=\lambda_0+\lambda^{\alpha}\langle X_{\alpha}\rangle+\lambda^{\alpha\beta}\langle X_{\alpha}X_{\beta}\rangle+\cdots\\&=\lambda_0+\lambda^{\mu}{}_0G^{\alpha}{}_{\mu}\langle X_{\alpha}\rangle_0+\lambda^{\mu\nu}{}_0G^{\alpha}{}_{\mu}G^{\beta}{}_{\nu}\langle X_{\alpha}X_{\beta}\rangle_0+\cdots\\&=S_0+S_1+S_2+\cdots\ .\end{aligned} \tag{5.61}$$

The subscript zero on the expectation values denotes with respect to the reference state ρ_0.

We already know that the entropy is conserved. The new result we now prove is that each partial entropy S_i in (5.61) is separately conserved. Each set of powers of generators homogeneous of degree n evolves separately with its very own conserved entropy. In essence this is a direct result of the closure properties (5.57) and (5.58).

The partial entropy of degree n is defined by

$$S_n\equiv-\mathrm{Tr}[\rho A_n(t)]\ , \tag{5.62}$$

where

$$\begin{aligned}A_0(t)&=\lambda_0(t)I\ ,\\A_1(t)&=\lambda^{\alpha}(t)X_{\alpha}\ ,\\A_2(t)&=\lambda^{\alpha\beta}(t)X_{\alpha}X_{\beta}\ ,\end{aligned} \tag{5.63}$$

etc., and the (time-dependent) coefficients are given by (5.60). Using the automorphisms (5.56) and (5.57) it follows immediately that

$$U^{\dagger}A_n(t)U=A_n(0) \tag{5.64}$$

and hence that

$$\begin{aligned}S_n&=-\mathrm{Tr}[\rho A_n(t)]=-\mathrm{Tr}[U\rho_0U^{\dagger}A_n(t)]\\&=-\mathrm{Tr}[\rho_0U^{\dagger}A_n(t)U]=-\mathrm{Tr}[\rho_0A_n(0)]\ .\end{aligned} \tag{5.65}$$

The observables given by (5.63) are thus time-dependent constants of (our approximation to the) motion. Each one such "moment" is, for a reversible evolution, a carrier of its own entropy.

VI. EXAMPLE

To illustrate the method described, we consider a simple, nontrivial algebraic Hamiltonian: the forced Morse oscillator,[34] written in terms of the SU(2) generators. Our purpose is to present the abstract ideas of Secs. III—V in a concrete setting.

A. The Hamiltonian and the relevant algebra

The forced Morse oscillator describes, more realistically than the simple harmonic oscillator, a molecule or a vibrational nucleus, acted upon by an external time-dependent force. The force can be taken as due to the perturbation induced by a structureless particle moving along a classical trajectory. The one-dimensional Morse potential

$$V(r)=V_0(e^{-2a(r-r_0)}-2e^{-a(r-r_0)}) \tag{6.1}$$

provides a realistic description of experimental spectra.[36]

This potential was written previously[36] in algebraic terms by the generators of SU(2) $\{J_0,J_1,J_2\}$. The group[28] SU(2), being isomorphic to the rotation group in three di-

mensions O(3), has the commutation relations of angular momentum:

$$[J_l,J_m]=i\epsilon_{lmn}J_n,\quad l,m,n=0,1,2 \tag{6.2}$$

where ϵ_{lmn} is the three-dimensional, completely antisymmetric tensor. It is convenient to introduce the other basis $\{J_\pm,J_0\}$ where

$$J_\pm=J_1\pm iJ_2\ . \tag{6.3}$$

The Morse oscillator Hamiltonian is now written as[36]

$$H_0=A(J_-J_++J_0)=A(J^2-J_0^2)\ . \tag{6.4}$$

$J^2=J_1^2+J_2^2+J_0^2$ is the Casimir operator for SU(2), and is considered as a constant within an irreducible representation of the algebra.

The external force is written as

$$V(t)=if(t)(J_++J_-)=2f(t)J_1 \tag{6.5}$$

in terms of the same generators. The full Hamiltonian is then $H=H_0+V(t)$.

The Hamiltonian H_0 is nonlinear in the generators and is therefore not closed under commutation relations with them:

$$\begin{aligned} &i[H_0,J_0]=0\ ,\\ &i[H_0,J_1]=-A(J_0J_2+J_2J_0)\ ,\\ &i[H_0,J_2]=A(J_0J_1+J_1J_0) \end{aligned} \tag{6.6}$$

for the force $V(t)$ the commutation relations are

$$\begin{aligned} &i[V,J_0]=-2f(t)J_2\ ,\\ &i[V,J_1]=0\ ,\\ &i[V,J_2]=2f(t)J_1\ . \end{aligned} \tag{6.7}$$

The natural relevant observables, which form a Lie algebra, are the three generators of SU(2).

B. The reference state

The reference state is chosen as one with maximal entropy with respect to H_0 (that is, J_0^2 and J_0) as the original constraint, that is,

$$\rho_0=e^{(-\lambda_0-\beta H_0)}=e^{(-\lambda_0-\beta AJ^2-\lambda^1J_0-\lambda^2J_0^2)}\ , \tag{6.8}$$

where the Lagrange multipliers $\lambda_0,\lambda^1,\lambda^2$ are determined as usual by

$$\begin{aligned} &\mathrm{Tr}\rho_0=1\ ,\\ &\mathrm{Tr}\rho_0J_0=\langle J_0\rangle_0\equiv j_0\ ,\\ &\mathrm{Tr}\rho_0J_0^2=\langle J_0^2\rangle\equiv jj_0\ . \end{aligned} \tag{6.9}$$

The stability group of ρ_0 is clearly the one-dimensional subgroup U(1) with the generator J_0:

$$[\rho_0,J_0]=0\ . \tag{6.10}$$

The elements of the stability group are just the exponentials

$$h(\gamma)=e^{i\gamma\,\mathrm{Adj}J_0}$$

or

$$h(\gamma)A=e^{i\gamma\,\mathrm{Adj}J_0}A=e^{i\gamma J_0}Ae^{-i\gamma J_0} \tag{6.11}$$

(using the Baker-Hausdorff expansion) and $\mathrm{Adj}X_\mu A\equiv[X_\mu,A]$.

We now use the product representation of the group SU(2), which is[28] just the familiar Euler angles representation of the rotation group O(3):

$$U(\alpha,\beta,\gamma)=e^{i\alpha J_0}e^{i\beta J_2}e^{i\gamma J_0}\ . \tag{6.12}$$

The first advantage of this representation becomes clear when we apply it to ρ_0 to get ρ as in (5.1):

$$\rho=e^{i\alpha J_0}e^{i\beta J_2}e^{i\gamma J_0}\rho_0e^{-i\gamma J_0}e^{-i\beta J_2}e^{-i\alpha J_0}$$

or

$$\rho(\alpha,\beta)=e^{i\alpha J_0}e^{i\beta J_2}\rho_0e^{-i\beta J_2}e^{-i\alpha J_0}\ , \tag{6.13}$$

where we have used (6.10). The parametrization of the two-dimensional quotient space SU(2)/U(1) is now clearly the two angles (α,β), and these are going to play the role of the canonical coordinate chart.

C. The symplectic structure

Consider first the derivatives (5.13):

$$\begin{aligned} \frac{\partial\rho}{\partial\alpha}&=i(J_0\rho-\rho J_0)=i[J_0,\rho]\ ,\\ \frac{\partial\rho}{\partial\beta}&=ie^{i\alpha J_0}e^{i\beta J_2}[J_2,\rho_0]e^{-i\beta J_2}e^{-i\alpha J_0}\\ &=i[J_2\cos\alpha+J_1\sin\alpha,\rho]\ , \end{aligned} \tag{6.14}$$

where we have used over and over again the inner automorphisms of SU(2) as given in Appendix B. Comparing (6.14) with (5.13) identifies the transformation,

$$\begin{aligned} &\hat{J}_0=J_0\ ,\\ &\hat{J}_1=J_2\cos\alpha+J_1\sin\alpha \end{aligned} \tag{6.15}$$

and

$$\begin{aligned} \hat{\sigma}_{\mu0}&=\frac{\partial\langle J_\mu\rangle}{\partial\alpha}=i\,\mathrm{Tr}\rho[J_\mu,J_0]\ ,\\ \hat{\sigma}_{\mu1}&=\frac{\partial\langle J_\mu\rangle}{\partial\beta}=i\,\mathrm{Tr}\rho[J_\mu,J_2\cos\alpha+J_1\sin\alpha]\ , \end{aligned} \tag{6.16}$$

from which the symplectic structure is easily derived:

$$\sigma_{\mu\nu}=\begin{bmatrix} 0 & \langle J_1\rangle\cos\alpha-\langle J_2\rangle\sin\alpha\\ -\langle J_1\rangle\cos\alpha+\langle J_2\rangle\sin\alpha & 0 \end{bmatrix}. \tag{6.17}$$

The expectation values of the generators,

$$\begin{aligned} \langle J_\mu\rangle&=\mathrm{Tr}\rho(\alpha,\beta)J_\mu=\mathrm{Tr}U(\alpha,\beta)\rho_0U^\dagger(\alpha,\beta)J_\mu\\ &=\mathrm{Tr}\rho_0U^\dagger(\alpha,\beta)J_\mu U(\alpha,\beta)\ , \end{aligned} \tag{6.18}$$

can be written explicitly in terms of α,β and the initial (at

ρ_0) expectation values, by using again the automorphisms of Appendix B:

$$\begin{aligned}\langle J_0\rangle &= \mathrm{Tr}\rho J_0 = \mathrm{Tr}\rho_0 J_0\cos\beta + \mathrm{Tr}\rho_0 J_1 \sin\beta\ ,\\ \langle J_1\rangle &= \mathrm{Tr}\rho J_1 = \mathrm{Tr}\rho_0 J_0\cos\alpha\cos\beta - \mathrm{Tr}\rho_0 J_1 \sin\alpha\cos\beta\\ &\quad + \mathrm{Tr}\rho_0 J_0\cos\alpha\sin\beta\ ,\\ \langle J_2\rangle &= \mathrm{Tr}\rho J_2 = \mathrm{Tr}\rho_0 J_0\sin\alpha\sin\beta - \mathrm{Tr}\rho_0 J_1\sin\alpha\cos\beta\\ &\quad + \mathrm{Tr}\rho_0 J_2\cos\alpha\ .\end{aligned} \tag{6.19}$$

After taking into account the special form, (6.8), of ρ_0, we can write (6.19) as

$$\begin{aligned}\langle J_0\rangle &= j_0\cos\beta\ ,\\ \langle J_1\rangle &= -j_0\cos\alpha\sin\beta\ ,\\ \langle J_2\rangle &= j_0\sin\alpha\sin\beta\ .\end{aligned} \tag{6.20}$$

Inserting this relation into (6.18)

$$\sigma_{\mu\nu} = -j_0\sin\beta\begin{bmatrix}0 & 1\\ -1 & 0\end{bmatrix},\qquad \sigma^{\mu\nu} = -\frac{1}{j_0\sin\beta}\begin{bmatrix}0 & -1\\ 1 & 0\end{bmatrix}. \tag{6.21}$$

The matrix $\sigma_{\mu\nu}$ is nonsingular whenever $j_0\neq 0$, and $\sin\beta\neq 0$.

D. The equations of motion

To get the form of the equations of motion (5.34) we must write the Hamiltonian expectation value $H(\alpha,\beta) = \mathrm{Tr}(\rho H)$ in terms of α and β. That is,

$$\begin{aligned}H(\alpha,\beta) &= \mathrm{Tr}\rho H_0 + \mathrm{Tr}\rho V\\ &= \mathrm{Tr}\rho_0[U^\dagger(\alpha,\beta)H_0U(\alpha,\beta)\\ &\quad + U^\dagger(\alpha,\beta)VU(\alpha,\beta)]\ ,\end{aligned} \tag{6.22}$$

$$\begin{aligned}H_0 &= A\ \mathrm{Tr}\rho(J_1^2+J_2^2) = A\ \mathrm{Tr}\rho(J^2-J_0^2)\\ &= A[j(j+1) - jj_0\cos^2\beta - jj_1\sin^2\beta]\end{aligned} \tag{6.23}$$

and is independent of α. We used the fact that

$$\begin{aligned}&\langle J_0J_1 + J_1J_0\rangle_0 = 0,\quad jj_1 \equiv \langle J_1^2\rangle_0\ ,\\ &V(\alpha,\beta) = 2f(t)\langle J_1\rangle = -2j_0f(t)\cos\alpha\sin\beta\ .\end{aligned} \tag{6.24}$$

The full reduced Hamiltonian is then

$$\begin{aligned}H(\alpha,\beta) &= A[j(j+1) - jj_0\cos^2\beta - jj_1\sin^2\beta]\\ &\quad - 2j_0f(t)\cos\alpha\sin\beta\ .\end{aligned} \tag{6.25}$$

We are now in a position to write the equation of motion for α and β:

$$\dot\alpha = -\frac{1}{j_0\sin\beta}\frac{\partial H}{\partial\beta} = A\frac{2(jj_1-jj_0)}{j_0}\cos\beta + 2f(t)\cos\alpha\cot\beta\ , \tag{6.26}$$

$$\dot\beta = \frac{1}{j_0\sin\beta}\frac{\partial H}{\partial\alpha} = 2f(t)\sin\alpha\ .$$

One can verify these equations by calculating alternatively the expectation values,

$$\mathrm{Tr}\rho i[H,J_\mu]\ , \tag{6.27}$$

and then using (6.6), (6.7), and (6.15) to get the same equations.

The equations (6.26) are simple but nonlinear equations and the solution is not necessarily periodic. Their actual solution is discussed in Sec. VI F below.

Using the relations (6.20), one can give the equations for the expectation values:

$$\begin{aligned}\frac{\partial\langle J_0\rangle}{\partial t} &= j_0\sin\beta\,\dot\beta\left[= -\frac{\partial H}{\partial\alpha} = -2j_0f(t)\cos\alpha\sin\beta\right],\\ \frac{\partial\langle J_1\rangle}{\partial t} &= +j_0\sin\beta\sin\alpha\,\dot\alpha - j_0\cos\beta\cos\alpha\,\dot\beta\ ,\\ \frac{\partial\langle J_2\rangle}{\partial t} &= j_0\sin\beta\cos\alpha\,\dot\alpha + j_0\cos\beta\sin\alpha\,\dot\beta\ .\end{aligned} \tag{6.28}$$

The last two equations can now be written as

$$\cos\alpha\frac{\partial\langle J_2\rangle}{\partial t} + \sin\alpha\frac{\partial\langle J_1\rangle}{\partial t} = \frac{\partial H}{\partial\beta} \tag{6.29}$$

as expected from Eqs. (5.35) and (6.15).

E. The self-consistent Hamiltonian

From the definition (5.40) we can now write the linear self-consistent Hamiltonian $\mathcal{H}$

$$\begin{aligned}\mathcal{H}(\alpha,\beta) &= \dot\alpha\hat J_0 + \dot\beta\hat J_1\\ &= AJ_0\frac{2(jj_1-jj_0)}{j_0}\cos\beta\\ &\quad + f(t)(2J_0\cos\alpha\cot\beta + J_2\sin 2\alpha - 2J_1\sin^2\alpha)\ .\end{aligned} \tag{6.30}$$

This Hamiltonian is by no means a simple linearization of the original quadratic (in the generators) Hamiltonian. However, it gives the same values of the "relevant velocities" when taken inside the trace with ρ.

F. Stability analysis and computational results

The equations (6.26) for the group parameters have fixed points for $\sin\alpha = 0$ and $\cos\beta = 0$, for which $\dot\alpha = \dot\beta = 0$. The equations are, however, singular when $\sin\beta = 0$, near which $\cot\beta\to\infty$. In order to examine the stability of the equations near these fixed points we must find the roots of the characteristic equation.

The fixed points are $\alpha = n\pi$, $\beta = \pi/2 + m\pi$ for all integer n,m. The roots are determined by the determinant

$$\begin{vmatrix}-2f\cos\alpha\cot\beta - s & -2g\sin\beta - 2f\cos\alpha\dfrac{1}{\sin^2\beta}\\ 2f\cos\alpha & -s\end{vmatrix} = 0\ , \tag{6.31}$$

where $g \equiv A(jj_1 - jj_0)/j_0$ is a negative constant and

$f=f(t)$ is the acting known force. The roots of this equation at the fixed points are given by

$$s_{1,2}=\pm 2[-f(f+(-1)^{n+m}g)]^{1/2}\ . \tag{6.32}$$

For a small (compared to g) force all the fixed points are elliptic (when two roots are purely imaginary[37]) and therefore stable. Otherwise, half of the points become hyperbolic fixed points (when the two roots are real and of opposite sign[37]) near which the system becomes unstable.

Figure 1 shows typical behavior. The initial state is thermal [as in (6.8), with $\beta A=0.2$ and $j=60$ which are the values for a typical molecule at about 1000 K]. The three panels are for the force

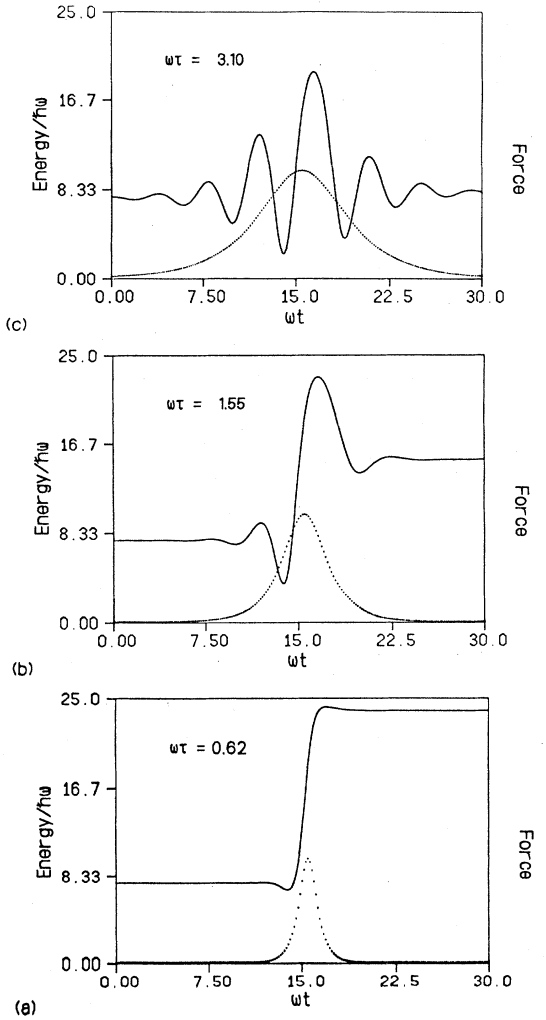

FIG. 1. Energy of a Morse oscillator [in units of the harmonic frequency (Ref. 36) $\hbar\omega$] vs time (solid line). Energy varies with time due to the action of an external force [shown as a dotted line, cf. (6.33)]. Three cases are shown: (a) the near sudden limit ($\omega\tau=0.62$) where the energy transfer to the oscillator is high (Ref. 38), (b) a post-resonant case ($\omega\tau=1.55$), and (c) an almost adiabatic forcing ($\omega\tau=3.10$), with a low net energy transfer. Increasing $\omega\tau$ even further results in a nearly completely adiabatic process where the oscillator fully adjusts to the external force and as $t\to\infty$ returns to its initial state.

$$f(t)=f/\cosh(t/\tau) \tag{6.33}$$

at three values of the "width" τ [smaller, about equal and larger than the harmonic period $2\pi/\omega$ of the oscillator $\omega=A(j+2)$]. Shown is the time dependence of the force and of the mean energy of the oscillator. At resonance ($\omega\tau=1$) the oscillator is significantly excited. For $\omega\tau<1$ the perturbation is very nearly sudden while for $\omega\tau>1$ the response of the oscillator is adiabatic as it adjusts to the force. This is as expected on physical grounds.[38]

VII. SUMMARY

Closed equations of motion of Hamiltonian form are derived for the mean values of a set of relevant observables used to describe the system. The mean values determine, via the maximal entropy formalism, a time-dependent density matrix for the system. The resulting time propagation is shown to be self-consistent. In general the procedure yields a variational approximation but can provide an exact description under well-defined conditions. The time evolution is reversible in that the entropy does not increase and that it can be described by a unitary evolution operator. (The extension to dissipative processes is in preparation for publication.) From a formal point of view, the reversible case is shown to correspond to a "completely integrable" time evolution in the reduced phase space. The exact time evolution is always reversible and the proposed approach can indeed yield exact results—when exact time-dependent constants of the motion can be constructed.[33] Here we deal with a variational approximation to such constants. Since such approximate constants can often be phenomenologically identified[39] or constructed on the basis of intuitive models, one typically has a good starting point for the selection of the relevant observables. A special case of both practical and formal importance is when the relevant observables form a Lie algebra. The constants of the motion (including the self-consistent Hamiltonian) are then linear in the generators. Moreover, a wide class of initial states can then be handled and the self-consistency condition can be implemented by solving differential (rather than functional) equations. To conclude, we have provided a time-dependent mean field variational formulation for the phenomenological procedures of surprisal analysis.

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APPENDIX A: THE MATRIX $D_\mu{}^\nu$ FOR THE TWO POSSIBLE PARAMETRIZATIONS OF THE GROUP

In order to derive the explicit form of the matrix $D_\mu{}^\nu$ in (5.12) we write (5.10) and (5.11) in detail:

$$\frac{\partial U(\xi)}{\partial \xi^\nu}=\frac{\partial}{\partial \xi^\nu}e^{+i\xi^\mu X_\mu}$$
$$=i\int_0^1 dx\, e^{ix\xi^\mu X_\mu}X_\nu e^{i(1-x)\xi^\mu X_\mu}$$
$$=i\int_0^1 dx\, e^{i(1-x)\xi^\mu X_\mu}X_\nu e^{ix\xi^\mu X_\mu}\,, \tag{A1}$$

where we used the explicit form for the derivative of an exponential operator.[27] If we now define

$$\hat{X}_\nu(\xi)=i\int_0^1 dx\, e^{ix\xi^\mu X_\mu}X_\nu e^{-ix\xi^\mu X_\mu} \tag{A2}$$

we get

$$\frac{\partial U}{\partial \xi^\nu}=i\hat{X}_\nu U,\quad \frac{\partial U^\dagger}{\partial \xi^\nu}=-iU^\dagger\hat{X}_\nu\,. \tag{A3}$$

Equation (A2) is known as the Kubo transform[40] of X_ν with the parameters ξ. Using the Baker-Hausdorff expansion[28]

$$e^{iA}Be^{-iA}=B+i[A,B]+\tfrac{1}{2}i^2[A,[A,B]]+\cdots \tag{A4}$$

and the closure property of the algebra (5.2) we see that (A2) is indeed an operator of the algebra. The transformation (A2) maps a basis of the algebra $\{X_\mu\}$ into another basis $\{\hat{X}_\mu\}$, because the inner automorphisms,

$$g(\xi)X_\mu g^{-1}(\xi),\ g\in G \tag{A5}$$

always do so. The matrix $D_\mu{}^\nu(\xi)$ is thus nonsingular and can be explicitly evaluated using the Kubo transform (A2) and the commutation relation (5.2).

For the product representation[26]

$$U(\eta)=\prod_\lambda e^{i\eta^\lambda X_\lambda}=e^{i\eta^1X_1}\cdots e^{i\eta^mX_m} \tag{A6}$$

and (in reversed order)

$$U^\dagger(\eta)=\prod_\lambda e^{-i\eta^\lambda X_\lambda}=e^{-i\eta^mX_m}\cdots e^{-i\eta^1X_1} \tag{A7}$$

we easily see

$$\frac{\partial U}{\partial \eta^\nu}=e^{i\eta^1X_1}\cdots iX_\nu e^{i\eta^\nu X_\nu}\cdots e^{i\eta^mX_m}$$
$$\equiv i\hat{X}_\nu\prod_\lambda e^{i\eta^\lambda X_\lambda}=i\hat{X}_\nu U(\eta) \tag{A8}$$

and similarly

$$\frac{\partial U^\dagger}{\partial \eta^\nu}=-e^{-i\eta^mX_m}\cdots e^{-i\eta^\nu X_\nu}iX_\nu\cdots e^{-i\eta^1X_1}$$
$$=-ie^{-i\eta^mX_m}\cdots e^{-i\eta^1X_1}\hat{X}_\nu=-iU^\dagger(\eta)\hat{X}_\nu\,. \tag{A9}$$

$\hat{X}_\nu$ and the matrix $D_\mu{}^\nu(\eta)$ are thus determined solely from the well-known automorphisms (no summation)

$$e^{i\eta^\lambda X_\lambda}X_\nu e^{-i\eta^\lambda X_\lambda}\,. \tag{A10}$$

For this case, no integration is needed.

APPENDIX B: THE INNER AUTOMORPHISMS OF SU(2)

We have

$$e^{i\alpha J_0}J_1e^{-i\alpha J_0}=J_1\cos\alpha-J_2\sin\alpha\,, \tag{B1}$$
$$e^{i\alpha J_0}J_2e^{-i\alpha J_0}=J_2\cos\alpha+J_1\sin\alpha\,, \tag{B2}$$
$$e^{i\beta J_2}J_0e^{-i\beta J_2}=J_0\cos\beta-J_1\sin\beta\,, \tag{B3}$$
$$e^{i\beta J_2}J_1e^{-i\beta J_2}=J_1\cos\beta+J_0\sin\beta\,, \tag{B4}$$
$$e^{i\gamma J_1}J_2e^{-i\gamma J_1}=J_2\cos\gamma-J_0\sin\gamma\,, \tag{B5}$$
$$e^{i\gamma J_1}J_0e^{-i\gamma J_1}=J_0\cos\gamma+J_2\sin\gamma\,. \tag{B6}$$

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