PHYSICAL REVIEW A VOLUME 35, NUMBER 5 MARCH 1, 1987

General dynamical invariants for time-dependent Hamiltonians

E. Duering, D. Otero, A. Plastino, and A. N. Proto
Departamento de Física, Comisión Nacional de Energía Atómica, avenida del Libertador 8250, 1429 Buenos Aires, Buenos Aires, Argentina
and Departamento de Física, Facultad de Ciencias Exactas, Universidad Nacional de la Plata, Casilla de Correo 67, 1900 La Plata, Buenos Aires, Argentina
(Received 6 August 1986)

Invariants for quantal or classical Hamiltonians are derived via the information-theory form of the statistical operator $\hat{\rho}$ which satisfy the maximum-entropy principle. The invariants can be constructed even for nonlinear time-dependent Hamiltonians, and recourse to the statistical operator allows for the possibility of ascribing a thermodynamical meaning to our invariants.

I. INTRODUCTION

More than twenty years have elapsed since Jaynes[1] pioneered the information-theoretic approach to statistical mechanics. Up to now many authors[2-4] have worked on several applications of these ideas. Recent studies[5-7] allow for a connection between the maximum-entropy principle and quantum theory, giving rise to a suggestive combination of macroscopic and microscopic concepts. As examples we can cite the connection found between information theory and Ehrenfest's theorem[7] and the possibility of expressing usual thermodynamical relationships in terms of the expectation values of quantal operators.[8] In particular, the Onsager coefficients can be easily rederived from the Hamiltonian of the system.[8] Of course, the entropy is a broadly used quantity in thermodynamics, although to regard it using it as a quantum dynamical quantity is not often seen in the literature.[1-8]

It is the aim of this paper to exploit the results obtained by Lewis and Leach (Ref. 9) in order to generate dynamical invariants for any given Hamiltonian H, of which the entropy S is just a special case. The existence of constants of motion (or invariants for shorting) is a point of central importance in the study of dynamical systems.[10-13]

If a sufficient number of invariants can be given, the motion can be described without a direct integration of the equations of motion. In this sense, previous works[10-13] (and the references therein show) a great variety of ingenious methods to deal with time-dependent, nonlinear or integrable (or even mixtures of these different types) Hamiltonians. The method that we present here was not devised as an alternative route for dealing with integrable Hamiltonians. Our aim is that of understanding the meaning of our invariants in connection with statistical or thermodynamical properties of systems. The present approach can be applied both to classical or to quantal Hamiltonians

$$\hat{H}=\sum_n h_n(\langle \hat{A}_n \rangle_t,t)\hat{A}_n$$

with $h_n(\langle \hat{A}_n \rangle_t,t)$ any function of t and of the mean values $\langle \hat{A}_n \rangle_t$ (where the subindex t, indicates the temporal dependence of $\langle \hat{A}_n \rangle$). We introduce explicitly these mean values to indicate possible nonlinearities of the Hamiltonian.

In Sec. II we present an extension of the usual IT formalism especially suited for our present purposes and several examples are discussed in Sec. III and some conclusions are drawn in Sec. IV.

II. AN EXTENDED INFORMATION-THEORY FORMALISM

It is well known that the main tool is given by a density matrix operator defined as[2,5,7]

$$\hat{\rho}=\exp\left[-\lambda_0-\sum_j^M \lambda_j(t)\hat{O}_j\right], \tag{2.1}$$

where $\hat{O}_j$ are the M "relevant" operators (in the sense of Ref. 15) that include $\hat{O}_0\equiv\hat{1}\equiv$identity operator and the Lagrange multipliers λ_j are determined as usual.[4,5,7] The operators $\hat{\rho}(t)$ and $\ln\hat{\rho}(t)$ obey, respectively,[5] the equations of motion

$$i\hbar\frac{\partial\hat{\rho}}{\partial t}=[\hat{H}(t),\hat{\rho}(t)] \tag{2.2a}$$

and

$$i\hbar\frac{\partial \ln\hat{\rho}}{\partial t}=[\hat{H}(t),\ln\hat{\rho}(t)], \tag{2.2b}$$

making it easy to verify[5,7] that the relevant operators are those that close a partial Lie algebra under commutation with the Hamiltonian $\hat{H}$

$$(i\hbar)^{-1}[H(t),O_j]=\sum_{i=0}^M g_{ij}\hat{O}_i, \tag{2.3}$$

where the g_{ij} are the structure constants of a partial lie algebra. Additionally the temporal equation for the λ's is given by

$$\frac{d}{dt}\lambda_i=\sum_l g_{il}\lambda_l, \tag{2.4}$$

which is easily obtained using Eqs. (2.2), (2.5), and (2.7).

The temporal evolution of the $\langle \hat{O}/\hat{\rho}\rangle$ as function of the initial conditions, are given by[5] (in matrix form)

$$\langle \hat{O}/\hat{\rho} \rangle_t = \tilde{F} \langle \hat{O}/\hat{\rho} \rangle_t \quad (2.5)$$

where $\tilde{F}$ denotes the transpose of a square matrix F defined by

$$-\frac{\partial F}{\partial t} = F \cdot g \quad (2.6)$$

and

$$\hat{O}(t) = \tilde{F}\hat{O}(t_0) \ . \quad (2.7)$$

Besides the Lagrange multipliers obey

$$\lambda(t) = G\lambda(t_0) \quad (2.8)$$

with

$$G^{-1} = F \ . \quad (2.9)$$

In Eqs. (2.5), (2.6), and (2.8), $\langle \hat{O}/\hat{\rho} \rangle_t$, $\hat{O}(t)$, $\lambda(t)$, and $\lambda(t_0)$ represent (one) column matrices. The formalism is valid for classical Hamiltonian if conmutation relations are replaced by Poisson brackets. The formalism is also valid for nonlinear time-dependent Hamiltonians, as we shall demonstrate below.

Using the fact that any function of $\hat{\rho}$ is an invariant [in particular, $(\ln\hat{\rho})^n$] we deduce without any difficulty the additional invariants

$$\begin{aligned} I^{(n)} &= \langle (\ln\hat{\rho})^n/\hat{\rho} \rangle - (\langle \ln\hat{\rho}/\hat{\rho} \rangle)^n \\ &= I_1^{(n)} - I_2^{(n)} \ , \end{aligned} \quad (2.10)$$

with

$$I_1^n = \langle (\ln\hat{\rho}/\hat{\rho})^n \rangle \ , \quad (2.11)$$

$$I_2^n = (\langle \ln\hat{\rho}/\hat{\rho} \rangle)^n \ . \quad (2.12)$$

For the particular case $n=2$, (2,10) takes the interesting form

$$I^{(2)} = \sum_{1,j=0}^{M} \lambda_r \lambda_j K_{rj} \ , \quad (2.13)$$

where K_{rj} is the so-called "centered" correlation coefficient[8] $(\langle \frac{1}{2}[\hat{A}_r,\hat{A}_j]_+ \rangle - \langle \hat{A}_r \rangle \langle \hat{A}_j \rangle)$. We can also use, in some cases, noncentered coefficients $K_{rj}^0 = \langle \frac{1}{2}[A_r,A_j]_+ \rangle$.

The correlation coefficients are evaluated using a $\hat{\rho}$ density matrix constructed with the $\{\hat{O}_i\}$ operator set and with their expectation values, which are usually the measured information at our disposal. Then it is possible to obtain the temporal evolution of the K's from the knowledge of the evolution of the λ's and $\langle O_r \rangle$'s, by recourse to the relationship

$$I^n(t) = I^n(t_0) \quad (2.14)$$

as was done in Ref. 7 with the entropy S. This procedure requires only that we solve a set of N coupled equations for the λ's.[6,7] More generally, we may assert that the time evolution of any function of $\hat{O}_j$ which accepts a series expansion can be obtained in terms of the $K^{(n)}$'s. The invariants constitute a generalization of those obtained by[9–12] and in Sec. III we shall give some illustrative examples.

In the following sections we shall restrict ourselves to $n=2$ invariants that have been widely used before.[10–13] We begin by introducing a matricial notation for the invariants. It is obvious that Eq. (2.13) involves bilinear products of Lagrange multipliers and operators, which can be conveniently expressed by introducing the Kronecker direct product[13]

$$\Lambda^{(2)} = \lambda \otimes \lambda \ , \quad (2.15)$$

$$\hat{K}^{(2)} = \hat{O} \otimes \hat{O} \quad (2.16)$$

(where both λ and $\hat{O}$ are column matrices). The temporal evolution of $\Lambda^{(2)}$ and $\hat{K}^{(2)}$ is given by [using Eqs. (2.7) and (2.8)]

$$\Lambda^{(2)}(t) = [G \times G]\Lambda^{(2)}(t_0) = [G]_2\Lambda^{(2)}(t_0) \quad (2.17)$$

and

$$\hat{K}^{(2)}(t) = [F \times F]\hat{K}^{(2)}(t_0) = [F]_2\hat{K}^{(2)}(t_0) \ , \quad (2.18)$$

so that

$$\hat{K}^{(2)}(t)\Lambda^{(2)}(t) = \hat{K}_0^{(2)}[F]_2[G]_2\Lambda_0^{(2)} = \hat{K}_0^{(2)}\Lambda_0^{(2)} \ , \quad (2.19)$$

where the subscript 0 corresponds to t_0. We see that $\hat{K}\Lambda$ is a secular invariant. To obtain Eq. (2.19) we have used vectors. However, the same result can be obtained using square matrices, with additional advantages that we shall discuss below. Then

$$\Lambda^{(2)} = \{\lambda_i, \lambda_j\} \ , \quad (2.20)$$

$$\hat{K}_1^{(2)} = \{[\hat{O}_i, \hat{O}_j]_+\} \ , \quad (2.21)$$

with

$$\hat{K}_2^{(2)} = \tfrac{1}{2}[\hat{O}_i, \hat{O}_j]_+ - \langle \hat{O}_i \rangle \langle \hat{O}_j \rangle \quad (2.22)$$

and

$$\hat{K}_3^{(2)} = \tfrac{1}{2}[\hat{O}_i, \hat{O}_j]_+ - \langle \hat{O}_j \rangle \hat{O}_i - \langle \hat{O}_j \rangle \hat{O}_j \ , \quad (2.23)$$

where Eqs. (2.22) and (2.23) represent different possible "realizations"[14] of the correlation operator defined previously. Now, the temporal evolution is given by

$$\Lambda^{(2)}(t) = G\Lambda_0^{(2)}\tilde{G} \quad (2.24)$$

and

$$\hat{K}^{(2)}(t) = \tilde{F}\hat{K}^{(2)}(t)F \ . \quad (2.25)$$

Equations (2.24) and (2.25) can be easily verified in terms of Eqs. (2.7) and (2.8). Combining Eqs. (2.24) and (2.25) we obtain

$$\Lambda^{(2)}(t)\hat{K}_t^{(2)} = G\Lambda_0^{(2)}\hat{K}_0^{(2)}F = G\Lambda_0^{(2)}\hat{K}_0^{(2)}G^{-1} \ . \quad (2.26)$$

Equation (2.26) represents a similarity transformation. This means that the matrix $\Lambda\hat{K}$ can be diagonalized and the coefficients of the secular equation are invariants. Then, $\mathrm{Tr}(\Lambda\hat{K})$, the corresponding determinant and its complementary minors are, *all of them,* invariant quantities. In particular,

$$I^{(2)} = \mathrm{Tr}(\Lambda\hat{K}) \ . \quad (2.27)$$

However, only one eigenvalue of $\Lambda^{(2)}$ is different from zero, so that the determinant and its minors carry no information whatsoever. Only the trace [Eq. (2.27)] remains as a nontrivial invariant, as was previously shown. As a general comment, it is interesting to remember that the Λ and K spaces are generated by the carrier spaces[14] of the λ's and the O's, and that the properties of the former are determined by those of the latter.

As pointed out before, the operators entering in the definition of $K^{(2)}$ are those which fulfill Eq. (2.3). This means that they are the relevant operators related to the Hamiltonian of the system. For any of them we can use Ehrenfest's theorem

$$\frac{\partial\langle\hat{O}\rangle}{\partial t}=(i\hbar)^{-1}\langle[\hat{H},\hat{O}]\rangle+\left\langle\frac{\partial O}{\partial t}\right\rangle , \tag{2.28}$$

and, using the definition (2.23), we are led to

$$[\hat{H},\hat{K}_{rj}]=i\hbar\left[\sum_l g_{lr}(\hat{K}_{ls}-\langle\hat{O}_l\rangle\hat{O}_j)+\sum_l g_{lj}(\hat{K}_{lr}-\langle\hat{O}_l\rangle\hat{O}_r)\right] . \tag{2.29}$$

At first sight, the $\hat{K}$'s defined by Eq. (2.27) do not close an algebra with $\hat{H}$. This is not a consequence of the structure of the $\hat{K}$'s, but a result of working with centered operators. Now, in using Eq. (2.28) for the $\hat{K}$'s and applying again Ehrenfest's theorem for the $\langle\hat{O}_j\rangle$ we obtain [cf. Eq. (2.29)]

$$\frac{\partial}{\partial t}\langle\hat{K}_{rj}\rangle=\sum_l(g_{lr}\langle\hat{K}_{lj}\rangle+g_{lj}\langle\hat{K}_{lr}\rangle) . \tag{2.30}$$

This result is valid for any definition of the $\hat{K}$ operators. Equation (2.15) and (2.16) lead to

$$\frac{\partial}{\partial t}\Lambda_{rj}=\frac{\partial\lambda_r\lambda_j}{\partial t}=\sum_l(g_{jl}\lambda_r\lambda_l+g_{rl}\lambda_j\lambda_l) , \tag{2.31}$$

while Eq. (2.30) and (2.31) can be written in matrix form as

$$-\dot{\hat{K}}=\tilde{g}\cdot\hat{K}+\hat{K}\cdot g , \tag{2.32}$$

where $\tilde{g}$ is the transpose of the g matrix defined in Eq. (2.3) and, further,

$$\dot{\Lambda}=g\cdot\Lambda+\Lambda\cdot\tilde{g} . \tag{2.33}$$

Equations (2.32) and (2.33) are the temporal equations for the $\hat{K}$'s and the Λ's in terms of the "old" g matrix. They are equivalent to Eq. (2.28), and give the dynamics of Λ and of $\hat{K}$ as a function of the old g matrix, obtained from Eq. (2.3).

Further properties of the vectorial spaces λ, and $\hat{O}$ can be obtained by defining the scalar product[15]

$$\hat{O}e\hat{O}=\text{ invariant} , \tag{2.34}$$

where e is the metric of the vectorial space defined by the O vector. The e matrix is determined by Eq. (2.34) and it follows that

$$Fe\tilde{F}=e . \tag{2.35}$$

In Eq. (2.35) the F matrix is such that the e matrix is nontrivial, so that the closure relation is fulfilled. It is possible to derive Eq. (2.35) ($\dot{e}=0$) obtaining

$$\dot{F}e\tilde{F}=-Fe\dot{\tilde{F}} \tag{2.36}$$

or using Eq. (2.6)

$$ge=-e\tilde{g} \tag{2.37}$$

although for time-dependent Hamiltonians it should be kept in mind that $\dot{e}=0$, so as to fulfill Eq. (2.34).

The e matrix obtained from Eq. (2.35) contains all the invariants that can be constructed with the $\hat{O}_i$ with respect to the given $\hat{H}$, as all the Hamiltonian dynamics is contained in the g (or in either F, or G) matrix.

Let us now construct the matrix[15]

$$\underline{eKeK}=\underline{\mathcal{K}}=\underline{K}^t\underline{K}_t . \tag{2.38}$$

The temporal evolution of $\mathcal{K}$ is given by [using Eq. (2.25)]

$$\begin{aligned}\underline{K}^t\underline{K}_t&=\underline{eK}(t)\underline{eK}(t)=\underline{eFK}(t_0)\underline{FeFK}(t_0)\underline{F}\\&=\underline{eFK}(t_0)\underline{eK}(t_0)\underline{F}\\&=\underline{F}^{-1}\underline{eK}(t_0)\underline{eK}(t_0)\underline{F} .\end{aligned} \tag{2.39}$$

Then $\mathcal{K}(t)$ relates to $\mathcal{K}(t_0)$ through a similarity transformation. As before, Tr $\mathcal{K}$, det $\mathcal{K}$, and its complementary are dynamical invariants, then

$$\text{Tr}\mathcal{K}=\text{ invariant}=K_tK^t , \tag{2.40a}$$

$$\det\mathcal{K}=\text{ invariant}=(\det K)^2 , \tag{2.40b}$$

where the upper (lower) label t implies a covariant (contravariant) tensorial character.[15]

This is a typical quantal result, and derives from the uncertainty relation. This kind of invariants *have not been derived before,* although for some Hamiltonians the determinant was found to be an invariant of motion[16] (but not the trace). In Sec. III we shall give some examples on this procedure.

III. EXAMPLES OF TIME-DEPENDENT INVARIANTS

We present in this section several examples that exhibit the usefulness of the extended IT formalism just introduced. Some elementary problems are summarized in Table I (free particle, harmonic oscillator, and the Larmor precession), besides which we develop the following nontrivial examples.

A. The time-dependent harmonic oscillator

As an example we review here some results referred to Ref. 17, which assumes the existence for a time-dependent harmonic oscillator, of the invariant $I(t)$ given below. The Hamiltonian is

$$\hat{H}=\frac{1}{2M}[\hat{p}^2+\omega^2(t)\hat{q}^2] \tag{3.1}$$

TABLE I. Some examples and application of the extended IT formalism.

H	$\hat{O}_i$	g	e	$\hat{O}_t\hat{O}^t$
$\frac{p}{2m}$	$\hat{q},\hat{p}$	$\begin{bmatrix} 0 & 0 \\ -1/m & 0 \end{bmatrix}$	$\begin{bmatrix} 0 & e_{12} \\ -e_{12} & e_{22} \end{bmatrix}$	$e_{12}[\hat{q},\hat{p}]+e_{22}\hat{p}^2$
$\frac{p2}{2m}+\frac{m}{2}\hat{q}^2$	$\hat{q},\hat{p}$	$\begin{bmatrix} 0 & m^2 \\ -1/m & 0 \end{bmatrix}$	$\begin{bmatrix} 0 & e_{12} \\ -e_{12} & 0 \end{bmatrix}$	$e_{12}[\hat{q},\hat{p}]$
$\frac{-eB}{2mc}S_Z$	S_x,S_y	$\begin{bmatrix} 0 & -\frac{-eB}{2mc} \\ \frac{eB}{2mc} & 0 \end{bmatrix}$	$\begin{bmatrix} e_{11} & e_{12} \\ -e_{12} & e_{11} \end{bmatrix}$	$e_{12}[S_x,S_y]+e_{11}(S_x^2+S_y^2)$

and $I(t)$ reads

$$I(t)=\tfrac{1}{2}\{\alpha(t)\hat{q}^2+\beta(t)\hat{p}^2+\gamma(t)[\hat{q},\hat{p}]_+\}\ , \tag{3.2}$$

where $[\ ]_+$ is the anticommutator of $\hat{p}$ and $\hat{q}$. In applying our formalism we can close the algebra (with H) with the following operators sets: $\{\hat{O}_0,\hat{q},\hat{p}\}$, $\{\hat{O}_0,\hat{q}^2,\hat{p}^2\hat{L}\}$, or $\{\hat{O}_0,\hat{q}^2,\hat{p}^2,\hat{q},\hat{p},\hat{L}\}$. Thus, our invariants are

$$I_1(t)=\lambda_0^{(1)}+\lambda_1^{(1)}(t)\langle\hat{q}\rangle_t+\lambda_2^{(1)}(t)\langle\hat{p}\rangle_t\ , \tag{3.3}$$

$$I_2(t)=\lambda_0^{(2)}+\lambda_1^{(2)}\langle\hat{q}^2\rangle_t+\lambda_2^{(2)}(t)\langle\hat{p}^2\rangle_t +\lambda_3^{(2)}(t)\langle\hat{L}\rangle_t\ , \tag{3.4}$$

$$I_3(t)=\lambda_0^{(3)}+\lambda_1^{(3)}(t)\langle\hat{q}\rangle_t+\lambda_2^{(3)}(t)\langle\hat{p}\rangle_t +\lambda_3^{(3)}(t)\langle\hat{p}^2\rangle_t+\lambda_4^{(3)}(t)\langle\hat{q}^2\rangle_t+\lambda_5^{(3)}\langle\hat{L}\rangle_t\ , \tag{3.5}$$

where $\hat{L}=[\hat{q},\hat{p}]_+=\hat{q}\hat{p}+\hat{p}\hat{q}$.

In particular, Eq. (3.4) is equivalent to (3.2). Both $\lambda_1^{(2)}(t)$ and $\alpha(t)$, $\lambda_2(t)$ and $\beta(t)$, and $\lambda_3^{(3)}(t)$ and $\gamma(t)$ follow the same equations of motion [(2.4)]. This fact can be easily checked by a simple comparison of Eq. (2.4) with those appearing in Ref. 18.

B. Simple time-dependent Hamiltonians

Other Hamiltonians (see Ref. 10) such as

$$H=a(t)\hat{p}^2+b(\hat{q},t)\hat{p}+c(\hat{q},t) \tag{3.6}$$

can be also solved provided the terms $b(\hat{q},t)\hat{p}$ and $c(\hat{q},t)$ close an algebra with $\hat{H}$ in the sense of Eq. (2.3). Another interesting choice for b and c could be to equate them to the time-dependent temporal evolution of any of the operators involved in the closure relation. For example,

$$\hat{H}=a(t)\hat{p}^2+\langle\hat{q}\rangle_t\hat{p}+\langle\hat{L}\rangle_t\ . \tag{3.7}$$

The Hamiltonian of Eq. (3.6) closes an algebra with the sets $S_1=\{\hat{O}_0,\hat{q},\hat{q}^2,\hat{p}^2\}$ and $S_2=\{\hat{O}_0,\hat{q},\hat{p},\hat{q}^2,\hat{p}^2,\hat{L}\}$.

The corresponding g matrices are characterized by the following nonvanishing elements:

$$g_{01}^{(1)}=-\langle\hat{q}\rangle_t,\ \ g_{21}^{(1)}=-2a(t) \tag{3.8}$$

and

$$g_{01}^{(2)}=-\langle\hat{q}\rangle_t,\ \ g_{13}^{(2)}=-2\langle\hat{q}\rangle_t\ ,$$
$$g_{21}^{(2)}=-2a(t),\ \ g_{25}^{(2)}=-2\langle\hat{q}\rangle_t\ , \tag{3.9}$$
$$g_{45}^{(2)}=-4a(t),\ \ g_{53}^{(2)}=-2a(t)\ ,$$

respectively. With these g matrices, the temporal evolution of the λ's can be evaluated via Eq. (2.4) and $(\ln\hat{\rho})^n$ can thus be constructed.

Notice that due to the nonlinearity of the Hamiltonian, the integration of the λ's should be made numerically.

C. A boson Hamiltonian

Let us now consider the time-independent Hamiltonian

$$\hat{H}=\epsilon_1 a^\dagger a+\epsilon_2 b^\dagger b+V(a^\dagger b+b^\dagger a)\ , \tag{3.10}$$

TABLE II. Elements of the e matrix obtained via the use of Eq. (2.37).

e_{11}	e_{12}	$(e_{12}-e_{15})\frac{V}{\epsilon_1-\epsilon_2}$	0	e_{15}
e_{21}	e_{22}	e_{23}	e_{24}	$-\frac{\epsilon_1-\epsilon_2}{V}e_{23}+e_{22}-2e_{44}$
$(e_{21}-e_{51})\frac{V}{\epsilon_1-\epsilon_2}$	e_{32}	$e_{44}+\frac{V}{\epsilon_1-\epsilon_2}(e_{23}-e_{53})$	$\frac{\epsilon_1-\epsilon_2}{2V}e_{24}$	$e_{32}+e_{53}-e_{23}$
0	$-e_{24}$	$\frac{\epsilon_1-\epsilon_2}{2V}e_{24}$	e_{24}	e_{24}
e_{51}	$e_{22}-2e_{44}-\frac{\epsilon_1-\epsilon_2}{V}e_{32}$	e_{53}	$-e_{24}$	$-\frac{\epsilon_1-\epsilon_2}{V}(e_{53}+e_{32})+e_{22}$

where $a^\dagger, a$ are the creation and annihilation operators ($[a,a^\dagger]=1$, $[b,b^\dagger]=1$, $[a,b]=[a^\dagger,b]=[a,b^\dagger]=[a^\dagger,b^\dagger]=0$).

Applying Eq. (2.3) the operator set is $\{\hat{O}_0, \hat{N}_a=a^\dagger a;\ \hat{N}_{ab}=a^\dagger b+b^\dagger a;\ \hat{I}_{ab}=i(a^\dagger b-b^\dagger a),\ \hat{N}_b=b^\dagger b\}=A_i$, $i=0$ to 4. The g matrix has the nonvanishing elements

$$\begin{aligned} g_{13}&=-2V=-g_{43},\quad g_{23}=(\epsilon_1-\epsilon_2)\,,\\ g_{31}&=-V=-g_{34},\quad g_{32}=(\epsilon_1-\epsilon_2)\,. \end{aligned} \tag{3.11}$$

Using Eq. (2.37) the e matrix can be obtained. (It is shown in Table II.) Then, enacting Eq. (2.34), we obtain

$$\begin{aligned} O_t e\tilde{O}_t = {} & e_{11}\hat{O}_0+(e_{12}+e_{21})\left[\hat{N}_a+\frac{V}{\epsilon_1-\epsilon_2}\hat{N}_{ab}\right]+(e_{15}+e_{51})\left[\hat{N}_b-\frac{V}{\epsilon_1-\epsilon_2}\hat{N}_{ab}\right]+e_{22}(\hat{N}_a+\hat{N}_b)^2\\ & -e_{23}\frac{\epsilon_1-\epsilon_2}{V}\left[\hat{N}_a+\frac{V}{\epsilon_1-\epsilon_2}\hat{N}_{ab}\right]\left[\hat{N}_b-\frac{V}{\epsilon_1-\epsilon_2}\hat{N}_{ab}\right]+e_{24}\frac{\epsilon_1-\epsilon_2}{V}i\left[\hat{N}_a-\hat{N}_b+\frac{2V}{\epsilon_1-\epsilon_2}\hat{N}_{ab}\right]\\ & -e_{32}\frac{\epsilon_1-\epsilon_2}{V}\left[\hat{N}_b-\frac{V}{\epsilon_1-\epsilon_2}\hat{N}_{ab}\right](\hat{N}_a+\hat{N}_b)-e_{53}\frac{\epsilon_1-\epsilon_2}{V}\left[\hat{N}_b-\frac{V}{\epsilon_1-\epsilon_2}\hat{N}_{ab}\right]^2\\ & +e_{44}[-2(\hat{N}_a\hat{N}_b+\hat{N}_b\hat{N}_a)+\hat{N}_{ab}\hat{N}_{ab}+\hat{I}_{ab}\hat{I}_{ab}]\,. \end{aligned} \tag{3.12}$$

As the e_i's are independent all the coefficients between brackets or parentheses are themselves invariants. There exists also the possibility to make alternative assumptions for the e's, so as to obtain different linear combinations of the invariants appearing in Eq. (3.12).

D. Lewis's Hamiltonian

Another Hamiltonian that we can study is[12]

$$\hat{H}=\tfrac{1}{2}\hat{p}^2+\frac{\dot{b}(t)}{a(t)}\hat{q}-\left[\frac{\ddot{a}}{2a}\right]\hat{q}^2\,, \tag{3.13}$$

with $a(t)$ and $b(t)$ arbitrary functions. Applying Eq. (2.3) we obtain for the set of relevant quantal operators $\{\hat{O}_0,\hat{q},\hat{p}\}$, the following nonvanishing elements for the g matrix:

$$\begin{aligned} g_{21}&=-1\,,\\ g_{02}&=\frac{\dot{b}(t)}{a(t)}\,,\\ g_{12}&=-\frac{\ddot{a}(t)}{a(t)}\,. \end{aligned} \tag{3.14}$$

Inserting this into Eq. (2.34) or (2.35) we obtain

$$\hat{O}_t e\hat{O}_t=e_{11}\hat{O}_0+e_{33}2\hat{H}+e_{32}[\hat{p},\hat{q}]\,. \tag{3.15}$$

As the Hamiltonian is time dependent e_{33} should be equal to zero. We obtain

$$\hat{O}_t e\hat{O}_t=e_{11}\langle\hat{O}_0\rangle-e_{32}i\hbar\langle\hat{O}_0\rangle\,. \tag{3.16}$$

E. Hietarinta's Hamiltonian

Let us now considering the quantal Hamiltonian

$$\hat{H}=\tfrac{1}{2}\hat{p}_x^2+\tfrac{1}{2}\hat{p}_y^2+2\hat{y}\hat{p}_x\hat{p}_y-\hat{x} \tag{3.17}$$

similar to the classical one presented by Hietarinta[17] and also analyzed by Hall.[16]

In this case, the closure relation (2.7) cannot be fulfilled, and the number of operators tends to infinity. However, it is possible to find a recurrence form for the invariants, as we shall see below.

The relevant operator sets are

$$\text{(a)}\quad \hat{O}_0,\hat{x},\hat{p}_x,\hat{y}\hat{p}_y,\hat{p}_y^2,\hat{p}_y^2\hat{p}_x,\hat{p}_y^2\hat{p}_x^2,\hat{p}_y^2\hat{p}_x^3,\hat{p}_y^2\hat{p}_x^4,\ldots, \tag{3.18}$$

$$\text{(b)}\quad \hat{O}_0,\hat{y},\hat{y}\hat{p}_x,\hat{y}\hat{p}_x^2,\hat{y}\hat{p}_x^3,\ldots,\hat{y}\hat{p}_x^n,\hat{p}_y,\hat{p}_y\hat{p}_x,\hat{p}_y\hat{p}_x^2,\ldots,\hat{p}_y\hat{p}_x^n\,. \tag{3.19}$$

The e matrix is then an infinite one, but it is possible, with a little algebra, and using only the first file of the e matrix, to arrive at

$$\begin{aligned} \hat{O}_t\hat{O}^t = {} & e_{11}\hat{O}_0+e_{12}\left[2\hat{x}-4\hat{y}\hat{p}_y\hat{p}_x-\hat{p}_x^2+\cdots+\hat{p}_y^2\sum_{n=1}^{\infty}\frac{(2\hat{p}_x^2)^n}{n!}\right]\\ & +(e_{14}+e_{41})(\hat{y}\hat{p}_y-\hat{p}_y^2\hat{p}_x-\tfrac{4}{3}\hat{p}_y^2\hat{p}_x^3-\tfrac{16}{5}\hat{p}_y^2\hat{p}_x^5+\cdots)+(e_{15}+e_{51})(\hat{p}_y^2+2\hat{p}_y^2\hat{p}_x^2+2\hat{p}_y^2\hat{p}_x^4+\cdots)\,. \end{aligned} \tag{3.20}$$

The invariant coefficient of e_{12} and $(e_{15}+e_{51})$ could be expressed also as

$$e_{12}[-2\hat{H}+\hat{p}_y^2\exp(2\hat{p}_x^2)]=\text{ invariant },\qquad(3.21)$$

$$(e_{15}+e_{51})\hat{p}_y^2\exp(2\hat{p}_x^2)=\text{ invariant }.\qquad(3.22)$$

These invariants have been previously founded by Hall,[16] and have been regained here in order to show how our method works when Eq. (2.3) gives an infinite number of operators.

IV. CONCLUSIONS

Most problems of physical interest are too complicated to be tackled "exactly." The impossibility of finding exact solutions for the problem of many interacting particles has fostered the development of approximate and qualitative methods. Unfortunately, questions concerning the validity of these approximations are very difficult to answer and one is often referred to exactly solvable models.

A broadly employed approach to evaluate the dynamical properties of a given system is to determine its invariants. The main result of this paper can be summed up by saying that we present a method that enables one to construct *the most general dynamical invariants for a given system*, with the advantage of relating them to well-known statistical operators.

The general dynamical invariants we have presented in Sec. II have been constructed exploiting the particular nature of the information-theory statistical operator, $\hat{\rho}$, which, due to Eq. (2.3) contains, within the present context, all the available information about the system of interest.

For $n=2$ the general invariants of Eq. (2.10) can be expressed in terms of the usual quantal correlation coefficients. This case deserves special care, as these correlations describe essential features of the corresponding system.

In Sec. II, we pay special attention to the second-order invariants, due to their peculiar structure. We demonstrate that the $\{\lambda\}$ and $\{\hat{O}\}$ constitute "carrier spaces" of the Λ [see Eq. (2.15)] and $\hat{K}_{rj}$, respectively [Eq. (2.16)]. Further, introducing a metric matrix e, and using the dynamical properties of the F matrix [defined in Eq. (2.6)] we can find the invariance properties of the $\hat{K}$ or $\mathscr{K}$ [see Eq. (2.36)] matrices. Then, for the second-order case, we find two different classes of invariants: $I^{(2)}=\mathrm{Tr}(\Lambda\hat{K})$ and those directly related with the K matrix as $\det K$, $\mathrm{Tr}(\mathscr{K})$; if the e matrix has another form [satisfying Eq. (2.34)], other invariants (in fact, different relations between the elements of the K matrix) can be obtained. Of course, they do not contain new information, but this procedure constitutes the most general way of constructing invariants of motion. Summarizing we can say that the main results of our work are the following.

(a) Due to the IT context, the invariants we study here can be related to usual quantal correlations (in a general case to higher-order correlations). This fact allows us to relate our expressions to similar ones coming from thermodynamics (see, for example, Ref. 8).

(b) The formalism we present here is valid for time-dependent Hamiltonians.

(c) For the second-order case, we introduce the metric matrix which allows us to relate the $\{\lambda\}$ and $\{\hat{O}\}$ spaces to the Λ and K spaces.

Notice also that we are prescribing the way to construct invariants according to a well-defined procedure. *No process of inference is employed,* as done in some previous and pioneer work.[11]

As a final word, let us emphazise that we are not using IT here in the usual (Jaynes's) sense of working (in the best possible way) with *incomplete* information, but from a different perspective: that of employing the *relevant* information (for a given Hamiltonian) in order to deal with some aspects of the exact dynamics. Opposite to Jaynes philosophy, ours is that of finding the best way of discarding "irrelevant" information, rather than making do with the incomplete one.

ACKNOWLEDGMENTS

The authors wish to thank Mrs. Verónica Zunino for her assistance in the final stages of this work. Two of us, E. Duering and A. Plastino, acknowledge support by Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET), Argentina.

[1]E. T. Jaynes, Phys. Rev. **106** 620 (1957); **108**, 171 (1957).

[2]A. Katz, *Principles for Statistical Mechanics* (Freeman, San Francisco, 1967); A. Hobson, *Concepts in Statistical Mechanics* (Gordon and Breach, New York, 1971).

[3]R. Baierlin, *Atoms and Information Theory* (Freeman, San Francisco, 1967); R. C. Tolman, *The Principles of Statistical Mechanics* (Clarendon, Oxford, 1938).

[4]W. T. Grandy, Jr., Phys. Rep. **62**, 175 (1970).

[5]Y. Alhassid and R. D. Levine, J. Chem. Phys. **67**, 4321 (1977).

[6]Y. Alhassid and R. D. Levine, Phys. Rev. A **18**, 89 (1978).

[7]D. Otero, A. Plastino, A. N. Proto, and G. Zannoli, Phys. Rev. A **26**, 1209 (1982).

[8]E. Duering, D. Otero, A. Plastino, and A. N. Proto, Phys. Rev. A **32**, 3681 (1985).

[9]H. R. Lewis and P. G. L. Leach, J. Math. Phys. **23**, 2371 (1982).

[10]H. R. Lewis, Jr. and W. B. Reisenfeld, J. Math. Phys. **10**, 1458 (1969).

[11]H. R. Lewis and P. G. L. Leach, J. Math. Phys. **23**, 165 (1982).

[12]H. R. Lewis, Phys. Rev. Lett. **18**, 510 (1967); J. R. Ray, Phys. Rev. A **28**, 2603 (1983).

[13]A. N. Kolmogorov and S. V. Fomin, *Elementos dela Teoría de Funciones y del Análisis Funcional* (Mir, Moscow, 1975).
[14]R. Gilmore, *Lie Groups, Lie Algebras and Some of Their Applications,* (Wiley, New York, 1974).
[15]E. Duering, D. Otero, A. Plastino, and A. N. Proto, Phys. Rev. A **32**, 2455 (1985).
[16]G. Nicolis, Rep. Prog. Phys. **42**, 225 (1979); L. S. Hall, Phys. Rev. Lett. **54**, 614 (1985).
[17]J. Hietarinta, Phys. Lett. **96A**, 273 (1983).
[18]E. S. Hernandez and B. Remaud, Phys. Lett. **75A**, 269 (1980).