Statistical inference in non-Hamiltonian dynamics

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(Received 22 December 1982; revised manuscript received 16 April 1984)

We assume that the formal results of the maximum-entropy approach for the description of some quantal systems remain valid in the presence of a perturbation that cannot be formulated in terms of a Hamiltonian, if the dynamical laws for a convenient set of observables are known. As an example we study the harmonic motion of a quantal object coupled to a heat reservoir (a) reversibly and (b) irreversibly. In case (b), the data concerning the evolution of the individual fluctuations permit the construction of a density matrix for all times.

I. INTRODUCTION

Statistical inference methods based on information theory[1] have shown their relevance for a large variety of problems in physics, ranging from the interpretation of statistical mechanics and thermodynamics[2] to applications of molecular[3,4] and nuclear[5,6] collision problems, nuclear fission,[7] and quantum mechanics.[8] In spite of the diversity of systems under the focus of this type of description, most of them correspond to either thermal equilibrium or reversible dynamics. These are the processes governed by the Schrödinger—von Neumann or Liouville equation, where the density operator $\hat{\rho}$ varies in time as

$$\begin{aligned} i\dot{\hat{\rho}} &= [\hat{H},\hat{\rho}]/\hbar \\ &= L\hat{\rho} \end{aligned} \tag{1.1}$$

under the action of the known Hamiltonian $\hat{H}$ or the Liouvillian L. So far those dynamical problems that cannot be cast in the form (1.1) lie beyond the scope of these methods. Two main examples can be quoted.

One of them corresponds to an object that undergoes reversible motion, but the structure of its Hamiltonian is hidden from the observer, who suspects, after recording some expectation values of observables, that the real Hamiltonian differs slightly from a known one $\hat{H}_0$. The other example is the case of irreversible motion characterized by a non-Hamiltonian generator of the evolution.[9,10] Some of these situations have been dealt with in previous papers. In Refs. 11 and 12 a typical problem of master-equation dynamics has been approached but no general rule has been formulated. In Ref. 13 the treatment is based on the assumption that the measurable properties of the system under consideration experience slight deviations with respect to a set of unperturbed values, characteristic of the Schrödinger problem.[3,4,8]

Our aim here is to propose a different approach. We notice that statistical inference methods are founded on the hypothesis that a closed algebra of observables under commutation with the known Hamiltonian $\hat{H}_0$ does exist. This assumption cannot be maintained when the Hamiltonian is missing. In many cases of interest, however, a set of N observables $\hat{A}_r$, $r=1,\dots,N$, representing the measurable properties of the system, is available together with their equations of motion. We will assume in this paper that if these equations are "closed," in the sense that

$$\dot{A}_r = g_r(\{A_s\},t)\ , \tag{1.2}$$

where

$$A_r = \mathrm{Tr}(\hat{A}_r\hat{\rho})\ , \tag{1.3}$$

one can write a density matrix for arbitrary time t in the manner prescribed by information theory, with parameters that are given functions of t. It cannot be demonstrated, in general, that such a density matrix is the exact one for the given system. However, it is "exact" in the space of the observables $\{\hat{A}_r\}$ since it reproduces the expectation values $\{A_r\}$ as well as their linear functionals for arbitrary times t. Analytical functionals will be reproduced provided that dispersions and correlations remain small, i.e., quantities like $\mathrm{Tr}(\hat{A}_r^{n_r}\hat{A}_s^{n_s}\hat{\rho})$, for example, can be sensibly approximated by $A_r^{n_r}A_s^{n_s}$.

This paper is organized as follows. In Sec. II we briefly review the method of solution of the Schrödinger—von Neumann equation within the framework of information theory and present the formalism adequate for the generalization to dissipative evolution. Section III is devoted to the construction of the density matrix for the time-dependent harmonic oscillator (TDHO) using fluctuations and constants of the motion. We illustrate the problem of non-Hamiltonian dynamics examining, in this framework, a quantal harmonic oscillator coupled to a heat reservoir, whose master equation and properties of type (1.2) have been worked out in the literature.[14,15] This damped TDHO is investigated in Sec. IV, where the parameters characterizing the perturbed density matrix are evaluated as functions of time. Section V contains the final summary.

II. INTEGRATION OF THE TIME DERIVATIVE OF THE DENSITY OPERATOR

We assume that the system of interest, when isolated, is governed by an unperturbed Hamiltonian $\hat{H}_0$ and the overall dynamics can be referred to an algebra $\mathscr{A}$ of n observables $\hat{A}_r$, $r=1,\ldots,n$, plus the identity $\hat{A}_0=\hat{I}$, namely,

$$\mathscr{A}=\{\hat{A}_r \mid [\hat{H}_0,\hat{A}_r]=i\hbar\sum_s g_{rs}A_s\ ,\quad r=1,\ldots,n\}\ . \tag{2.1}$$

Hereafter we denote the set of $n+1$ operators by a vector $\hat{\vec{A}}=(\hat{A}_0,\ldots,\hat{A}_n)$. The structure of the algebra is contained in a matrix $\underline{G}$, i.e.,

$$[\hat{H}_0,\hat{\vec{A}}]=i\hbar\underline{G}\hat{\vec{A}}\ . \tag{2.2}$$

According to the Liouville equation (1.1) and the algebra definition (2.2), one can write the equation of motion for the c-numbers (1.3) as follows:

$$\dot{\vec{A}}=i\hbar(-\underline{G}\vec{A}+\underline{F}\vec{A})\ , \tag{2.3}$$

where $\underline{F}$ is the matrix accounting for the local variation of the operators $\hat{A}_r$.

Now, following Levine *et al.*,[3,4] hypothesis (2.3) allows one to write a solution for the Liouville equation in the form

$$\hat{\rho}^{(0)}(t)=\exp[-\vec{\lambda}^{(0)}(t)\cdot\hat{\vec{A}}(t)] \tag{2.4}$$

provided that the Lagrange multipliers included in the vector $\vec{\lambda}^{(0)}$ satisfy the equations of motion[3,4]

$$\dot{\vec{\lambda}}^{(0)}=(\underline{G}-\underline{F})^T\vec{\lambda}^{(0)}\ . \tag{2.5}$$

In several applications, as will be exemplified later in this work, it is convenient to resort to a slightly different way of expressing the solution of the unperturbed Liouville equation. Following Levine,[4,16] we introduce a set of m $(m\leq n)$ invariant operators or constants of the motion $\hat{J}_q$ linearly related to the $\hat{A}_r$'s,

$$\hat{\vec{J}}=\underline{C}\hat{\vec{A}}\ , \tag{2.6}$$

where $\underline{C}$ is an $m\times n$ matrix. The components of the vector $\hat{\vec{J}}$ are constants of the motion if

$$i\hbar\frac{d}{dt}\hat{\vec{J}}=i\hbar\frac{\partial}{\partial t}\hat{\vec{J}}+[\hat{\vec{J}},\hat{H}_0]=0\ . \tag{2.7}$$

If such a set exists, a solution of Eq. (1.1) is

$$\hat{\rho}^{(0)}(t)=\exp[-\vec{\alpha}\cdot\hat{\vec{J}}(t)]\ . \tag{2.8}$$

A straightforward calculation gives

$$\dot{\vec{\alpha}}(t)=\vec{0}\ . \tag{2.9}$$

Equations (2.4) and (2.8) must describe the same density matrix for given initial conditions. Thus the information measure given by $\ln\hat{\rho}(t)$ is unique and we have

$$\begin{aligned}\ln\hat{\rho}&=-\vec{\lambda}\cdot\hat{\vec{A}}\\&=-\vec{\alpha}\cdot\hat{\vec{J}}\ .\end{aligned} \tag{2.10}$$

This indicates that $\vec{\alpha}$ and $\vec{\lambda}$ are related by the matrix $\underline{C}$:

$$\vec{\alpha}=\underline{C}\vec{\lambda}\ . \tag{2.11}$$

We now consider the case in which the above-described system no longer is isolated, due to some coupling to the surroundings. To our current knowledge, this problem has not been formally approached with the help of information-based techniques, although there exist approaches in the sense of providing an ansatz[9,10] for the density matrix. Applications to molecular vibrational[9] and spin[10] relaxation have been worked for specific masterlike equations of motion. It is our intent to look for a prescription to extract a density matrix compatible with the available information, in the case in which the external coupling cannot be represented by a Hamiltonian.[17,18] Such a density matrix will approximate the exact one in the space of the operators that provide the available information. Regardless of the nature of the perturbation, we assume that our ignorance of the algebra for this new situation is compensated by the knowledge of the functions or c-numbers $A_r(t)$, or their equations of motion (1.2). These functions will be, in general, supplied by an experiment performed under given initial conditions. One should expect that, in most physical situations characterized by smooth, well-behaved parameters and laws of motion of the type of (1.2), the state of the perturbed system can be described by a formally invariant density matrix of the form (2.4) or (2.8). Some time dependence in the parameters $\alpha_r(t)$ makes room for the case in which the perturbation destroys the conservation of the mean value $\hat{\vec{J}}$, namely, when

$$\frac{d}{dt}\hat{\vec{J}}=\vec{f}(\hat{\vec{J}};t)\neq 0\ . \tag{2.12}$$

An example of such a situation will be analyzed in Sec. IV.

Now, we declare that we will not look for the exact solution $\hat{\rho}(t)$ of this non-Hamiltonian dynamics. To the extent to which most of the predictions expected when one studies a particular system depend on $\{A_r\}$ and on linear functionals and small dispersions of these observables, a density matrix like (2.4) or (2.8) will provide exact or very accurate solutions. Departures between the exact and the approximated density matrix will be significant if one becomes interested in the calculation of magnitudes involving high powers of $\{A_r\}$ and subsequent large dispersions. However, in many problems of interest a set of implicit equations for the derivatives of the parameters can be extracted from (2.4) and (1.2), giving

$$\vec{F}[\vec{\lambda}(t),\dot{\vec{\lambda}}(t)]=\vec{g}[\vec{A}(t),t]\ . \tag{2.13}$$

If the multipliers $\vec{\lambda}$ can be integrated out of this equation, the matrix composed of these coefficients reproduces the experimental evolution laws (1.2) for these observables by means of the formula[2–4]

$$\vec{A}=-\vec{\nabla}_{\vec{\lambda}}\lambda_0\ . \tag{2.14}$$

We will illustrate in detail the possibility of such a solution in Sec. IV.

III. UNDAMPED TIME-DEPENDENT HARMONIC OSCILLATOR

As a preliminary step to the examination of the damped TDHO, we extract in this section the relevant characteristics of the undamped problem. In this case the unperturbed Hamiltonian is

$$\hat{H}_0(t)=\frac{\hat{p}^2}{2m(t)}+\tfrac{1}{2}k(t)\hat{x}^2 . \tag{3.1}$$

According to some previous experience with this subject,[19,20] especially when dealing with the perturbed situations, we consider it useful to work with the centered, rather than the original, position and momentum operators,

$$\hat{X}=\hat{x}-x_0 , \quad x_0=\langle\hat{x}\rangle_0 \tag{3.2a}$$

$$\hat{P}=\hat{p}-\hat{p}_0 , \quad p_0=\langle\hat{p}\rangle_0 \tag{3.2b}$$

with the second moments

$$\chi_0=\langle\hat{X}^2\rangle_0 , \tag{3.3a}$$

$$\phi_0=\langle\hat{P}^2\rangle_0 , \tag{3.3b}$$

$$\sigma_0=\tfrac{1}{2}\langle\{\hat{X},\hat{P}\}\rangle_0 \tag{3.3c}$$

with { , } the usual anticommutator. These fluctuations are linked by the uncertainty relationship

$$\chi_0\phi_0-\sigma_0^2\geq\frac{\hbar^2}{4} . \tag{3.4}$$

A. Solutions of the Liouville equation

We select as the algebra $\mathscr{A}$ the set

$$\mathscr{A}=\{\hat{1},\hat{X},\hat{P},\hat{X}^2,\hat{P}^2,\{\hat{X},\hat{P}\}\} . \tag{3.5}$$

The matrices $\underline{G}$ and $\underline{F}$ of Eq. (2.3) are straightforwardly constructed as well as the set of equations (2.5) for the parameters that reads

$$\dot{\lambda}_0^{(0)}=0 , \tag{3.6a}$$

$$\ddot{\lambda}_i^{(0)}+\omega^2\lambda_i^{(0)}=0 , \quad i=1,2 \tag{3.6b}$$

$$\dot{\lambda}_3^{(0)}=2k\lambda_5^{(0)} , \tag{3.7a}$$

$$\dot{\lambda}_4^{(0)}=-\frac{2}{m}\lambda_5^{(0)} , \tag{3.7b}$$

$$\dot{\lambda}_5^{(0)}=-\frac{1}{m}\lambda_3^{(0)}+k\lambda_4^{(0)} . \tag{3.7c}$$

Comparing these equations with those displayed in Ref. 19 for the fluctuations, one sees that a solution of (3.7) is provided by

$$(\lambda_3^{(0)},\lambda_4^{(0)},\lambda_5^{(0)})=\frac{\alpha}{2}(\phi_0,\chi_0,-\sigma_0) , \tag{3.8}$$

where α is some proportionality constant. Thus if we let $\hat{J}_2$ be the quadratic invariant for the TDHO,[19]

$$\hat{J}_2=\tfrac{1}{2}(\phi_0\hat{X}^2+\chi_0\hat{P}^2-\sigma_0\{\hat{X},\hat{P}\}) , \tag{3.9}$$

and $\hat{J}_1$ the linear invariant[20]

$$\hat{J}_1=\lambda_1^{(0)}\hat{X}+\lambda_2^{(0)}\hat{P} , \tag{3.10}$$

in the most general case the density matrix is

$$\hat{\rho}^{(0)}(t)=\exp(-\alpha_0^{(0)}-\alpha_1^{(0)}\hat{J}_1-\alpha_2^{(0)}\hat{J}_2) , \tag{3.11}$$

with $\alpha_0^{(0)}$, $\alpha_1^{(0)}$, and $\alpha_2^{(0)}$ constant coefficients. We remark that the linear and quadratic invariants are the only constants of the motion for the TDHO. This assertion can be verified by straightforward calculation of the matrix $\underline{C}$ introduced in Eq. (2.6); as one imposes the conservation law given in (2.7), one sees that the equations for the elements of the matrix $\underline{C}$ possess two independent solutions, namely, one that gives rise to $\hat{J}_1$ and the other generating $\hat{J}_2$.

The determination of the density at any instant t demands the knowledge of the initial conditions for the Lagrange multipliers. Since the available data consist of the initial mean values of the algebra components $\{A_r(0)\}$, we must relate these to the parameters $\vec{\lambda}$ at $t=0$.

B. Canonical form of the density operator

Given a density matrix like (3.11), it reads, in the original algebra,

$$\hat{\rho}^{(0)}(t)=\exp(-\lambda_0^{(0)}\hat{1}-\lambda_1^{(0)}\hat{X}-\lambda_2^{(0)}\hat{P}-\lambda_3\hat{X}^2-\lambda_4^{(0)}\hat{P}^2-\lambda_5^{(0)}\{\hat{X},\hat{P}\}) . \tag{3.12}$$

We will next carry out a transformation on $\hat{\rho}^{(0)}$ that allows us to take advantage of standard results of statistical mechanics regarding the normalization. Once we know $\lambda_0^{(0)}$ as a function of $\lambda_1^{(0)}$–$\lambda_5^{(0)}$, Eq. (2.14) permits one to relate parameters to expectation values. Even though we are especially interested in these relationships at $t=0$ as discussed at the end of Sec. III A, it will be seen that they remain valid for arbitrary times.

A standard transformation in the space of the operators $\hat{X},\hat{P}$, actually a translation combined with a rotation, allows one to write the quadratic form in the exponent of (3.12) in its canonical representation. We obtain

$$\hat{\rho}^{(0)}=\exp(-\beta_0^{(0)}-\beta_1^{(0)}\hat{\xi}^2-\beta_2^{(0)}\hat{\eta}^2) . \tag{3.13}$$

The rotated variables $\hat{\xi}$ and $\hat{\eta}$ are given by the expressions

$$\hat{\xi}=a_0\left[\hat{X}+\hat{X}_0+\frac{\beta_1^{(0)}-\lambda_3^{(0)}}{\lambda_s^{(0)}}(\hat{P}+\hat{P}_0)\right] , \tag{3.14a}$$

$$\hat{\eta}=b_0\left[\hat{X}+\hat{X}_0+\frac{\beta_2^{(0)}-\lambda_3^{(0)}}{\lambda_5^{(0)}}(\hat{P}+\hat{P}_0)\right] , \tag{3.14b}$$

where the scaled factors a_0 and b_0 are

$$a_0=\lambda_5^{(0)}/[\lambda_5^{(0)2}+(\beta_1^{(0)}-\lambda_3^{(0)})^2]^{1/2} , \tag{3.15a}$$

$$b_0=\lambda_5^{(0)}/[\lambda_5^{(0)2}+(\beta_2^{(0)}-\lambda_3^{(0)})^2]^{1/2} , \tag{3.15b}$$

and the shift operators $\hat{X}_0$ and $\hat{P}_0$ possess the expectation values

$$\langle\hat{X}\rangle_0=\frac{\lambda_1^{(0)}\lambda_4^{(0)}-\lambda_2^{(0)}\lambda_5^{(0)}}{2\Delta^{(0)}} , \tag{3.16a}$$

$$\langle\hat{P}\rangle_0=\frac{\lambda_2^{(0)}\lambda_3^{(0)}-\lambda_1^{(0)}\lambda_5^{(0)}}{2\Delta^{(0)}} , \tag{3.16b}$$

with

$$\Delta^{(0)}=\lambda_3^{(0)}\lambda_4^{(0)}-\lambda_5^{(0)} . \tag{3.16c}$$

The Lagrange multipliers in the rotated frame are related to the older ones by

$$\beta_0^{(0)}=\lambda_0^{(0)}-\frac{\lambda_1^{(0)2}\lambda_4^{(0)}-2\lambda_1^{(0)}\lambda_2^{(0)}\lambda_5^{(0)}+\lambda_2^{(0)2}\lambda_3^{(0)}}{4\Delta^{(0)}} , \tag{3.17a}$$

$$\beta_{1,2}^{(0)}=\frac{\lambda_3^{(0)}+\lambda_4^{(0)}}{2}\pm\left[\left[\frac{\lambda_3^{(0)}+\lambda_4^{(0)}}{2}\right]^2-\Delta^{(0)}\right]^{1/2} . \tag{3.17b}$$

We notice that density (3.13) has the form of a thermal (Bloch) density related to a harmonic oscillator (HO) Hamiltonian $\hat{H}$,

$$\hat{\rho}_{\text{HO}}=\exp(-\alpha\hat{1}-\beta\hat{H}) , \tag{3.18}$$

if we properly identify the inertial and stiffness parameters of the latter. This amounts to defining

$$\beta_1^{(0)}=\beta\frac{K}{2} , \tag{3.19a}$$

$$\beta_2^{(0)}=\beta\frac{1}{2M} , \tag{3.19b}$$

and in this case we can profit from the following identification: let the inverse temperature β be represented by

$$\beta=\frac{\lambda_3^{(0)}+\lambda_4^{(0)}}{2} . \tag{3.20}$$

The frequency arises from (3.19) and (3.20) as

$$\Omega^2=\frac{16\Delta^{(0)}}{(\lambda_3^{(0)}+\lambda_4^{(0)})} \tag{3.21}$$

and the normalization can be found in standard text books[21] taking the form

$$\beta_0^{(0)}=-\ln\left[2\sinh\frac{\hbar\Omega\beta}{2}\right]$$

$$=-\ln[2\sinh(\beta_1^{(0)}\beta_2^{(0)})^{1/2}] . \tag{3.22}$$

The expressions of the Lagrange multipliers in terms of the current expectation values arise from the set of conditions, $\vec{\nabla}_{\beta^{(0)}}\beta_0^{(0)}=\langle\hat{\vec{A}}\rangle_0$, actually,

$$\langle\hat{\xi}\rangle_0=\langle\hat{\eta}\rangle_0=\langle\{\hat{\xi},\hat{\eta}\}\rangle_0=0 , \tag{3.23a}$$

$$\langle\hat{\xi}^2\rangle_0=-\frac{\partial\beta_0^{(0)}}{\partial\beta_1^{(0)}} , \tag{3.23b}$$

$$\langle\hat{\eta}^2\rangle_0=-\frac{\partial\beta_0^{(0)}}{\partial\beta_2^{(0)}} . \tag{3.23c}$$

The first two constraints give

$$\langle\hat{X}_0\rangle_0+\frac{\beta_1^{(0)}-\lambda_3^{(0)}}{\lambda_5^{(0)}}\langle\hat{P}_0\rangle_0=0 , \tag{3.24a}$$

$$\langle\hat{X}_0\rangle_0+\frac{\beta_2^{(0)}-\lambda_3^{(0)}}{\lambda_5^{(0)}}\langle\hat{P}_0\rangle_0=0 . \tag{3.24b}$$

Since $\beta_1\neq\beta_2$, it turns out that both $\langle\hat{X}_0\rangle_0$ and $\langle\hat{P}_0\rangle_0$ must vanish. According to (3.16) this means

$$\lambda_1^{(0)}=\lambda_2^{(0)}=0 . \tag{3.25}$$

In other words, no linear terms appear in the density (3.12). The remaining three constraints lead, after some algebra, to Eq. (3.8) with

$$\frac{2}{\alpha}=\frac{\hbar\langle\hat{J}_2\rangle_0^{1/2}}{\tanh^{-1}\left[\frac{\hbar}{2\langle\hat{J}_2\rangle_0}\right]} . \tag{3.26}$$

Recalling that $\hat{J}_2$ is an invariant operator, we realize that α is a constant. As anticipated at the beginning of this subsection, the relations given in Eq. (3.8) are valid at all times. Furthermore, the normalization λ_0 takes the form

$$\lambda_0^{(0)}=\frac{1}{2}\ln\frac{1}{4}\left[\frac{4\langle\hat{J}_2\rangle_0}{\hbar^2}-1\right] . \tag{3.27}$$

We can see that if $\langle\hat{J}_2\rangle_0$ takes its ground-state value $\hbar^2/4$, the parameters $\lambda_0^{(0)}$ and $\lambda_3^{(0)}-\lambda_5^{(0)}$ diverge. This behavior causes some uncertainty with respect to the boundedness of the matrix elements of the density operator $\hat{\rho}$. It is then worthwhile to perform an analysis measuring the lack of information, or entropy, in the vicinity of the singularity. With the variable

$$U=\left[\frac{4\langle\hat{J}_2\rangle_0}{\hbar^2}\right]^{1/2} \tag{3.28}$$

the entropy $S=-\text{Tr}(\hat{\rho}\ln\hat{\rho})$ reads

$$S(U)=-\ln 2+\tfrac{1}{2}\ln(U^2-1)+\tfrac{1}{2}U\ln\frac{U+1}{U-1} . \tag{3.29}$$

Regarded as a function of the real variable U, S vanishes when $U=1$ and increases as $\ln U$ when U approaches infinity. Furthermore, $S'(U)\geq 0$ indicates that $S(U)$ is a monotonic function. An analysis of $S(U)$ in the neighborhood of $U=1$ can be done as follows. Let

$$U=1+\delta \tag{3.30}$$

with $\delta\ll 1$. One finds

$$S\sim\frac{1+2\ln 2}{2}\frac{\delta}{2} . \tag{3.31}$$

Equation (3.31) indicates that in the vicinity of the ground state, namely when $\langle\hat{J}_2\rangle_0$ is slightly larger than $\hbar^2/4$, entropy and excess quantal uncertainty are, except for a scaling factor, equivalent measures of missing information. The preceding observation suggests a thermodynamic interpretation of Heisenberg uncertainty.

IV. DAMPED TIME-DEPENDENT HARMONIC OSCILLATOR

We now assume that the TDHO is coupled to its environments in such a way that its motion is no longer governed by a Hamiltonian. This problem has been described through different perturbative approaches[22] and various versions are available. In particular, in Refs. 14

and 15 the equations of motion for the fluctuations have been derived. Since these equations have been obtained from a master equation that rules the evolution of the density $\hat{\rho}(t)$,[14] they constitute a realization of Eq. (2.13). We will now illustrate the application of the method proposed in Sec. II to deal with these types of situations.

The formulas of interest are[14,15]

$$\dot{\chi}=\frac{2\sigma}{m}\ , \tag{4.1a}$$

$$\dot{\phi}=2(-\gamma\phi-k\sigma+D)\ , \tag{4.1b}$$

$$\dot{\sigma}=-k\chi+\frac{\phi}{m}-\gamma\sigma\ , \tag{4.1c}$$

where k and m are the parameters of the free Hamiltonian $\hat{H}_0$ [see Eq. (3.1)] and γ and D are the friction and diffusion coefficients, respectively, whose microscopic structure in terms of the coupling between the oscillator and the heat bath is given in Refs. 14 and 15. These four coefficients can be parametrized by arbitrary functions of time.[19]

If we propose that the density matrix of the perturbed TDHO is formally invariant, in other words, if it can be written in the form (3.12) or (3.13) with coefficients $\{\alpha_i(t)\}$ or $\{\lambda_i(t)\}$ different from $\{\alpha_i^{(0)}\}$ and $\{\lambda_i^{(0)}\}$, respectively, the equations of motion for the Lagrange multipliers are obtained as follows. From the formal invariance of $\lambda_0(t)$ and with the help of Eqs. (3.17), (3.22), and (3.25) we have

$$\lambda_0(t)=-\ln[2\sinh(\hbar\Delta^{1/2})]\ , \tag{4.2}$$

where

$$\Delta=\lambda_3\lambda_4-\lambda_5^2\ . \tag{4.3}$$

It turns out that the relationship between fluctuations and multipliers is the same as in Eq. (3.8) with $2/\alpha$ given by (3.26) after replacing the unperturbed value $\langle\hat{J}_2\rangle_0$ by the current one $\langle\hat{J}_2\rangle$. Opposite to the case in Sec. III, here $\hat{J}_2$ is no longer a constant of the motion. Its expectation value verifies an evolution law that can be extracted from Eqs. (4.1) and reads

$$\frac{d}{dt}\langle\hat{J}_2\rangle=-2\gamma\langle\hat{J}_2\rangle+2D\chi\ . \tag{4.4}$$

Taking the time derivatives of Eq. (3.8) and equating them with the data, namely Eqs. (4.1), we obtain a coupled differential system

$$\dot{\lambda}_i=\frac{d_i}{d}\ ,\quad i=3,4,5 \tag{4.5}$$

where

$$d_3=-\lambda_3^2bA-(1+2\lambda_5^2b-\lambda_3\lambda_4b)B+2\lambda_3\lambda_5bC\ , \tag{4.6a}$$

$$d_4=-(1+2\lambda_5^2b-\lambda_3\lambda_4b)A-\lambda_4^2bB+2\lambda_4\lambda_5bC\ , \tag{4.6b}$$

$$d_5=-\lambda_3\lambda_5bA-\lambda_4\lambda_5bB+(2\lambda_3\lambda_4b-1)\ , \tag{4.6c}$$

$$d=2\Delta b-1\ . \tag{4.6d}$$

We have here used the notation

$$A=-\frac{2\lambda_5}{m}\ , \tag{4.7a}$$

$$B=\frac{2D}{a}+2(k\lambda_5-\gamma\lambda_3)\ , \tag{4.7b}$$

$$C=k\lambda_4-\frac{\lambda_3}{m}-\gamma\lambda_5\ , \tag{4.7c}$$

and

$$b=\frac{1}{2\Delta}\left[1+\frac{2\hbar\Delta^{1/2}}{\sinh(2\hbar\Delta^{1/2})}\right]\ . \tag{4.7d}$$

Numerical integration of either the system (4.5) or the original one (4.1) for the underdamped and overdamped situations yield the results displayed in Figs. 1—4. In Fig. 1 we display the Lagrange multipliers $\alpha_0(t)$ and $\alpha_2(t)$ as functions of time, while the horizontal lines indicate the constant, unperturbed values $\alpha_0^{(0)}$ and $\alpha_2^{(0)}$. The period T of the free TDHO has been selected as the time unit, the damping coefficient equals $2T^{-1}$ and the diffusion coefficient takes the value $6T^{-1}$ throughout all calculations. In Fig. 2 we show the expectation value of $\hat{J}_2$, the proportionality parameter $2/\alpha$ in Eq. (3.26), the entropy S given in Eq. (3.29), and the quotient $\Delta=4\langle\hat{J}_2\rangle/\alpha^2$ for the same selection of coefficients. Figures 3 and 4 are the same as Figs. 1 and 2, respectively, but correspond to the overdamped oscillator with $\gamma=9T^{-1}$.

Let us first look at the odd-numbered graphs. We observe that the full, perturbed Lagrange multipliers α_0 and α_2 increase with opposite signs, α_0 being negative, and exceed the given scale at slightly more than $2T$. Their shape is quite similar, this fact being especially interesting

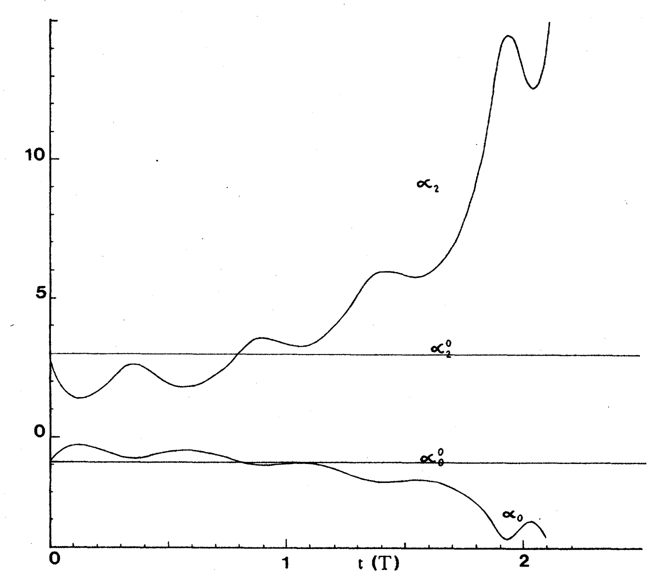

FIG. 1. The Lagrange multipliers α_0 and α_2 as functions of time (in units of the free period T) for the underdamped oscillator. Damping parameter is $\gamma=2T^{-1}$ and the diffusion coefficient is $D=6T^{-1}$. Horizontal lines indicate the perturbed values of the multipliers.

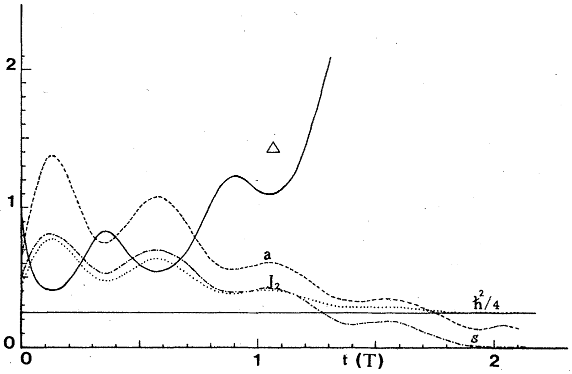

FIG. 2. Expectation value of the operator $\hat{J}_2$, the proportionality parameter $2/\alpha = a$, the quotient $\Delta = \langle \hat{J}_2 \rangle a^2$ and the entropy S as functions of time. Details are the same as in Fig. 1.

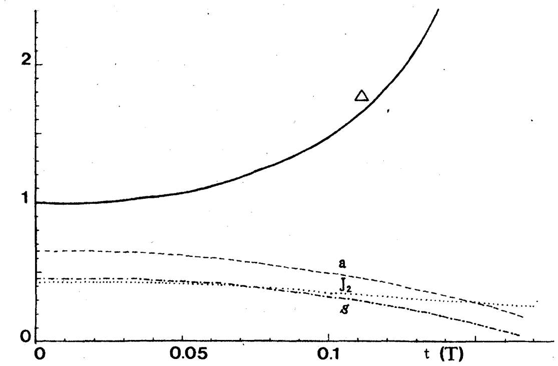

FIG. 4. Same as in Fig. 2 for the overdamped oscillator.

in the underdamped case (Fig. 1) where several oscillations can be observed. In spite of the divergent behavior that the parameters will attain as time keeps increasing, it can be seen that the density matrix remains a regular operator and, correspondingly, the entropy evolves towards a finite value. This statement can be proven as follows. In the even-numbered figures we can observe that the expectation value $\langle \hat{J}_2 \rangle$ moves towards an asymptote located at the value $\hbar^2/4$. In addition, we see that the divergence in the determinant Δ is related to the vanishing of the proportionality coefficient $2/\alpha(t)$. The evolution of $\langle \hat{J}_2 \rangle$ shows that the overall dynamics proceeds towards the singularity $U=1$ in the entropy that we have already discussed in Sec. III. Since we have seen that this is an avoidable singularity, the density matrix remains regular throughout the full evolution. This means that the opposite divergent behaviors of α_0 and α_2 compensate each other. Furthermore, the behavior of the entropy corresponds to the preceding comments and one observes that in either case it evolves towards an asymptotic zero value (cf. Sec. III). On first sight, this might seem to be in contradiction with well-known assertions of information theory and thermodynamics; however, in the present example the evolution has driven the system from an initially disordered mixed state at $t=0$ towards the nondegenerate ground state of the oscillator, namely, a pure state with zero entropy. Thus, according to thermodynamics, the amount of entropy released by the oscillator is a lower bound to the entropy production in the heat reservoir that provides the damping to the system under consideration.

One must recall that, as the unperturbed parameters $\alpha_0^{(0)}$ and $\alpha_2^{(0)}$ are constant, the exponential increase (decrease) in α_0 (α_2) affects the corrections $\alpha_i^{(1)} = \alpha_i - \alpha_i^{(0)}$, $i=1,2$. Although these shifts originate in the coupling which is analytically represented by the dissipative coefficients γ and D, they cannot be regarded as slight perturbations upon the parameters $\alpha_i^{(0)}$. This assertion holds even in the presence of a weak coupling between the oscillator and the heat reservoir; for example, in the underdamped situation present in Figs. 1 and 2, our results show that within 10—15 % of the period T, the amplitude of $\alpha_2^{(1)}$ reaches about one-half the unperturbed value of $\alpha_2^{(0)}$. We can observe, as well, in the odd-numbered figures that the shift departs from its initial zero value with a non-negligible slope. As a summary of this paragraph, we can say that the hypothesis of small deviations from the unperturbed multipliers can only be supported for very short, i.e., microscopic, times in the neighborhood of the origin.

Similar evolution patterns can be obtained for the separate fluctuations and multipliers. Opposite to the preceding case, the unperturbed fluctuations and multi-

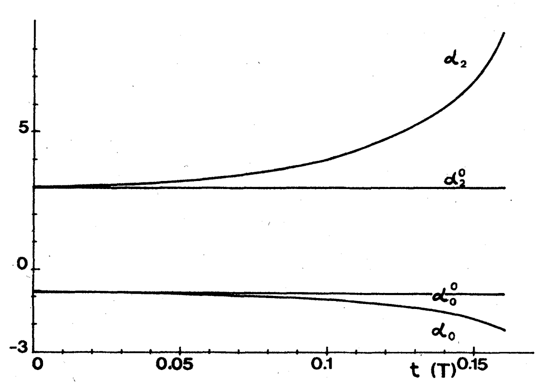

FIG. 3. Same as in Fig. 1 for the overdamped ($\gamma = 9T^{-1}$) oscillator .

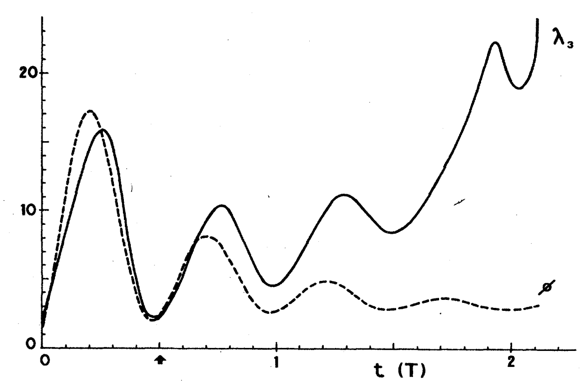

FIG. 5. Momentum dispersion ϕ (dashed line) and Lagrange multiplier λ_3 (solid line), for the underdamped ($\gamma = 2T^{-1}$) oscillator.

pliers are oscillating functions of time, rather than constants. An illustration of the type of results one can get is shown in Fig. 5, where we have drawn the dispersion ϕ and the parameter λ_3 for the underdamped case $\gamma=2/T$. The corresponding patterns for the unperturbed situation are sinusoidal with a period indicated by an arrow below the horizontal axis.

V. SUMMARY

In this work we have discussed the fact that in some problems of non-Hamiltonian dynamics, information-theory methods can be utilized to find an approximate density matrix that exactly reproduces the available data. We have assumed that, in general, one could look for a group of time-dependent Lagrange multipliers, provided that there exists a set of observables whose mean values evolve according to closed laws of motion. The possibility of such an approach in specific situations has been illustrated by studying a damped TDHO whose evolution is not driven by a Hamiltonian. Instead, we know the equations of motion for the fluctuations. In order to treat this problem with the approach proposed above it has been necessary to solve first the case of the free TDHO with the maximum-entropy formalism for the algebra of centered coordinate and momentum operators with respect to the unperturbed Hamiltonian.

It has been seen that the linear invariant $\hat{J}_1$ is irrelevant to the description of the TDHO, where the quadratic one $\hat{J}_2$ is equivalent to the complete algebra. A standard coordinate transformation carried on this operator permits one to calculate explicitly the Lagrange multipliers and to provide a thermodynamical interpretation of $\hat{J}_2$. In the case of the TDHO, we have assumed that the density matrix remains formally invariant and have found and solved the equations of motion for the shifted Lagrange multipliers.

Finally, we would like to stress here that, in general, one cannot assert that the "informational" density matrix of Eqs. (2.4) or (2.8) is the exact solution of any problem of irreversible motion. In the face of the need for the best solution of such a problem, our proposal presents the following advantages. First, it is a maximum-entropy density operator, i.e., $S[\hat{\rho}(t)]=-\mathrm{Tr}\hat{\rho}(t)\ln\hat{\rho}(t)$ is not smaller than $S[\hat{\sigma}(t)]$ for any density $\hat{\sigma}$ that does not possess the exponential structure.[3,4] Second, it reproduces exactly the experimental constraints and, of course, every linear combination of the set $\{\hat{A}_r\}$. Third, it provides the correct asymptotic or equilibrium solution, since $\hat{\rho}(0)$ is a maximum-entropy density. In particular, it is well known that in the case of a damped, time-independent harmonic oscillator, a Fokker-Planck equation rules the evolution of the density matrix.[14] The fluctuations of this density matrix obey equations of the motion of the type (4.1) and it has been shown[14] that the solution of the Fokker-Planck equation is exponentially quadratic. This exponent can be seen to be precisely our operator $\hat{J}_2$. This is then an example in which our proposal is the exact solution of the problem of irreversible motion. We believe that most generally, specific studies will be necessary in order to determine whether the maximum-entropy density matrix is the exact one for arbitrary non-Hamiltonian dynamics.

ACKNOWLEDGMENTS

The authors are indebted to the Laboratorio de Física del Plasma at the University of Buenos Aires for access to their computing facilities, and to their colleagues D. Otero, A. Plastino, and A. Proto for fruitful discussions. One of us (V.M.) acknowledges the Comisión de Investigaciones Científicas de la Provincia de Buenos Aires for support. One of us (E.S.H.) acknowledges the Consejo Nacional de Investigaciones Científicas y Técnicas for financial support. This work was performed under Grant No. 9413a/81 from CONICET, Argentina and No. 10030106-019 from SUBCYT, Argentina.

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