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Quantum Statistical Operator and Classically Chaotic Hamiltonian System

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Abstract

In a Hamiltonian system von Neumann Statistical Operator is used to tease out the quantum consequence of (classical) chaos engendered by the nonlinear coupling of system to its environment. An example of coupled oscillators is given. Such an operator, at fixed energy of system and at a given Poincaré section is in a mixed state, inevitably.

1.0 Introduction:

To every mechanical system there is a Hamiltonian function $H(p,q)$ (classical) or operator $H(-\frac{i\hbar d}{dq},q)$ (quantum), $p\in\mathbb{R}^n$, $q\in\mathbb{R}^n$, n∈ ℕ. Classically the Hamilton-Jacobi equations

$$\frac{dp_j}{dt} = -\frac{\partial H}{\partial q_j} \qquad (1i)$$

$$\frac{dq_j}{dt} = \frac{\partial H}{\partial p_j} \qquad (1ii)$$

$j=1,2,\dots,n,$ degrees of freedom *(dof)* spell the dynamics or the time (t) evolution of the system from classical state $(p(0),q(0))$ to classical state $(p(t),q(t))$ in phase space $(p,q)\subset\mathbb{R}^{2n}$. For any attribute $A(p,q)$ of the system, we also have

$$\frac{d}{dt}A = \sum_{j=1}^{n}\left(\frac{\partial A}{\partial q_j}\frac{\partial q_j}{dt} + \frac{\partial A}{\partial p_j}\frac{dp_j}{dt}\right) \quad (A \text{ not explicit in time } t)$$

which by eq.(1) means that

$$\frac{d}{dt}A = \sum_{j=1}^{n}\left(\frac{\partial A}{\partial q_j}\frac{\partial H}{\partial p_j} - \frac{\partial A}{\partial p_j}\frac{\partial H}{\partial q_j}\right) \equiv \{A,H\} \qquad (2)$$

the Poisson Bracket, PB of A and H. In particular $dH/dt = \{H,H\} = 0$, i.e. H is constant.
Usually system has ν functionally independent constants of motion (a.k.a. integrals of motion)

$$F_k(p,q) = C_k, \quad k=1,2,\dots,\nu \qquad (3)$$

For these,

$$0 = \frac{d}{dt}C_k = \frac{d}{dt}F_k(p,q) = \{F_k,H\} \qquad (4)$$

And since any $F_j(p,q)$ can serve as $H(p,q)$, $0=\frac{d}{dt}F_k = \{F_k,F_j\}$. Thus the ν F's must be (are said to be) in involution

$$\{F_j(p,q), \quad F_k(p,q)\} = 0, \; j,k=1,2,\dots,\nu \qquad (5)$$

And the system is integrable (superintegrable) if $\nu = n$ $(\nu > n)$. If $\nu < n$, system is <u>not</u> integrable or is nonintegrable; and if H is nonlinear and has bounded phase space, $|p|<\infty$, $|q|<\infty$, then system is (classically) chaotic. That is, its trajectory (solution of eq. (1)) in phase space is sensitively dependent on initial conditions, and practically equivalently has Lyapunov exponent $\lambda_L \epsilon \mathbb{R}_+$. Usually as a Hamiltonian system, $H(p,q) =$ constant E is necessarily a constant of motion (see above, $\frac{dH}{dt} = \{H,H\} = 0$). Hence $1 \le \nu < n$, and, as explained in Section 4, $n \ge 2$.
Nonintegrable systems are difficult analytically. Invariably one resorts to numerical solutions (cf Henon and Heiles (1964)).
A long time ago (1917) Einstein had remarked that Bohr's quantization prescription is for integrable (Hamiltonian) systems only (cf Gutzuiller (1990) and Lanezos (1949)). Similarly, under Schroedinger's prescription, $p\to -i\hbar\, d/dq$ or $q \to +i\hbar\, d/dp$, there is a great difficulty in dealing with non-integrable systems, quantum-mechanically, even conceptually because one does not have a complete set of observables.

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1. Quantum Mechanical Analysis

In quantum theory (cf Merzbacher, 1970) system is governed by $H(-i\hbar\frac{d}{dq}, q)$, (i.e. $p_j \equiv -i\hbar\,\partial/\partial q_j$) as system evolves from quantum state $|\psi(q,0)>$ to quantum state $|\psi(q,t)>$, spelt by the time-dependent Schroedinger Equation

$$\frac{i\hbar\partial}{\partial t}|\psi(q,t)> = H|\psi(q,t)> \qquad (6)$$

in the pertinent Hilbert space $\mathcal{H} \ni |\psi(q,t)>$. In the dual space, we have

$$-i\hbar\frac{\partial}{\partial t} < \psi(q,t)| = <\psi(q,t)|H^{+} = <\psi(q,t)|H \qquad (6')$$

H being self-adjoint. Given any relevant attribute $A(q,t)$ of the system, an observable, the expectation value of A in state $|\psi(q,t)>$ is

$$< A(q,t) >_{\psi} \equiv <\psi(q,t)|A(q,t)|\psi(q,t)> \qquad (7)$$

Usually there exists a basis $\{\varphi_m(q)\}_{m=1}^{M}$ of the pertinent Hilbert space with

$$<\varphi_r(q)|\varphi_s(q) \geq \delta_{rs} \qquad (8)$$

so that

$$|\psi(q,t)> = \sum_{m=1}^{M} c_m(t)|\varphi_m(q)>;\ c_m(t) \equiv <\varphi_m(q)|\psi(q,t)> \qquad (9)$$

in which case

$$< A(q,t) >_{\psi} = \sum_s\sum_r c_r^*(t) <\phi_r(q)|A(q,t)|\varphi_s(q)> c_s(t)$$
$$= \sum_s\sum_r c_r^*(t)c_s(t)a_{rs}(t) \qquad (10)$$

where

$$a_{rs}(t) \equiv <\varphi_r(q)|A(q,t)|\varphi_s(q)> \qquad (11)$$

Let us define density matrix $(M\times M)$

$$(\rho_\psi)_{sr} \equiv c_s^{(\mu)}(t)\,c_r^{(\mu)*}(t) \equiv \rho_{sr}^{(\mu)} \qquad (12)$$

Then

$$< A(q,t) >_{\psi} \equiv < A >^{(\mu)} = \sum_s\sum_r \rho_{sr}^{(\mu)}a_{rs}(t) = Tr\left[\rho^{(\mu)}a(t)\right] \qquad (13)$$

Suppose system can be in any of several quantum states $\{|\psi^{(\mu)}(q,t)>\}$. Then $< A >_{\psi}$ depends on μ and ρ_ψ is described as $\rho^{(\mu)}$, so that

$$< A >_{\psi} = < A >^{(\mu)} = Tr\left[\rho^{(\mu)}a(t)\right] \qquad (14)$$
$$\rho_{sr}^{(\mu)} = c_s^{(\mu)}\,c_r^{(\mu)*}$$

In a collection of such similar systems, let f_μ be the fraction of them that are in state $|\psi^{(\mu)}(q,t)>$, or the probability that system is in that state,

$$f_\mu \geq 0, \qquad \sum_{\mu=0}^{N} f_\mu = 1 \qquad (15)$$

the statistical average of attribute/observable $A(q,t)$ is given by

$$\ll A(q,t) \gg = \sum_\mu f_\mu < A >^{(\mu)} = \sum_\mu f_\mu\,Tr\left[\rho^{(\mu)}a(t)\right]$$
$$= Tr[\rho a(t)]$$

where

$$\rho = \sum_\mu f_\mu\,\rho^{(\mu)}, \qquad \rho_{sr} = \sum_\mu f_\mu\rho_{sr}^{(\mu)} \qquad (17)$$

Rho ρ is the (quantum), von Neumann statistical operator.

2. Features of von Neumann Statistical Operator.

(i) $\rho_{sr}^{(\mu)} = c_s^{(\mu)}\,c_r^{(\mu)*} = <\varphi_s(q)|\psi^{(\mu)}(q,t)><\psi^{(\mu)}(q,t)|\varphi_r(q)|>$

That is

$$\rho^{(\mu)} = |\psi^{(\mu)}><\psi^{(\mu)}|$$

Its adjoint

$$\rho^{(\mu)+} = \left|\psi^{(\mu)}><\psi^{(\mu)}\right| = \rho^{(\mu)}$$

That is, $\rho^{(\mu)}$ is self-adjoint, and hence $\rho = \sum_\mu f_\mu \, \rho^{(\mu)}$ is self-adjoint too.

(ii) Let λ_k be an eigenvalue of ρ, i.e. $\rho|\wedge_k\rangle = \lambda_k|\wedge_k\rangle$ in appropriate Hilbert space. Then

$$\lambda_k = \langle\wedge_k|\rho|\wedge_k\rangle$$
$$\lambda_k^* = \langle\wedge_k|\rho^+|\wedge_k\rangle = \langle\wedge_k|\rho|\wedge_k\rangle = \lambda_k \qquad (16)$$

That is, eigenvalue is real, as expected of a self-adjoint operator. Furthermore,

$$\lambda_k = \langle\wedge_k|\rho|\wedge_k\rangle = \langle\wedge_k| \sum_\mu f_\mu \, \rho^{(\mu)}|\wedge_k\rangle$$
$$= \sum_\mu f_\mu \langle\wedge_k|\psi^{(\mu)}\rangle\langle\psi^{(\mu)}|\wedge_k\rangle$$
$$= \sum_\mu f_\mu \langle\wedge_k|\psi^{(\mu)}\rangle\langle\wedge_k|\psi^{(\mu)}\rangle^*$$
$$= \sum_{\mu=0}^{N} f_\mu \, |\langle\wedge_k|\psi^{(\mu)}\rangle|^2 \geq 0. \qquad (17)$$

The eigenvalues are real and non-negative, and

$$\sum_{k=1}^{M} \lambda_k = Tr\rho = \sum_\mu f_\mu \sum_r \langle\varphi_r|\psi^{(\mu)}\rangle\langle\psi^{(\mu)}|\varphi_r\rangle$$
$$= \sum_\mu f_\mu \sum_r \langle\psi_r|\varphi_r\rangle\langle\varphi_r|\psi^{(\mu)}\rangle, \quad \sum_r |\varphi_{r\rangle\langle}|\varphi_r| = I$$
$$\sum_{k=0}^{M} \lambda_k \sum_{\mu=0}^{N} f_\mu \langle\psi^{(\mu)}|\psi^{(\mu)}\rangle = \sum_\mu f_\mu \;\; 1 = 1 \qquad (18)$$

(iii) $\rho^{(\mu)} \equiv |\psi^{(\mu)}\rangle\langle\psi^{(\mu)}| \equiv \sigma \equiv |\psi\rangle\langle\psi|$

$\sigma^2 = \sigma\sigma = |\psi\rangle\langle\psi|\psi\rangle\langle\psi| = |\psi\rangle\langle\psi| = \sigma$

Thus, with σ idempotent,

$$\sigma(\sigma - I) = 0 \qquad (19)$$

From eqs (17), (18), (19), we have the following:

σ is called a <u>pure</u> <u>state</u>, and has eigenvalues 1 and $(M-1)$ zeros, $1, 0,0,0, \ldots ,0$. That is if $f_\mu = \delta_{\mu\tau}$, then $\rho = \rho^{(\tau)}$ is a pure state, σ. Otherwise, the $\rho \equiv \sum f_\mu \rho^{(\mu)}$ is a <u>mixed</u> <u>state</u> and $\rho \neq \rho^2$, but of course its eigenvalues are real, non-negative and sum to 1.

(iv) Dynamics

(a) The statistical operator has a time evolution. Using eqs. (6) and (6′), we obtain

$$i\hbar\frac{\partial}{\partial t}\rho = i\hbar\frac{\partial}{\partial t}|\psi\rangle\langle\psi| - i\hbar\left|\psi\rangle\frac{\partial}{\partial t}\langle\psi\right|$$
$$= H|\psi\rangle\langle\psi| - |\psi\rangle\langle\psi|H = H\rho - \rho H$$
$$i\hbar\frac{\partial}{\partial t}\rho = -[\rho, H] \qquad (20)$$

(b) The statistical average has dynamics also.

$$i\hbar\frac{d}{dt} \ll A(q,t) \gg = i\hbar\frac{d}{dt}\, a(t)$$
$$= i\hbar\frac{d}{dt}\, Tr(A\rho) = i\hbar Tr\left[\frac{\partial A}{\partial t}\rho\right] + i\hbar\left[A\frac{\partial}{\partial t}\rho\right]$$
$$= i\hbar << \frac{\partial A}{\partial t} >> - Tr\big[A[\rho, H]\big]$$
$$TrA[\rho, H] = Tr[A\rho H] - Tr[AH\rho] = Tr[\rho HA - AH\rho]$$

Thus,

$$i\hbar\frac{d}{dt} \ll A(q,t) \gg = i\hbar << \frac{\partial A}{\partial t} >> + << [A, H] >> \qquad (21)$$

(v) Entropy

Whenever a statistical model is used, there is entropy.

$S/k \equiv -Tr[\rho \ln \rho]$ $\quad$ ($= 0$, if ρ is σ (pure))

where k is Boltzmann constant. This one seeks to extremize, subject to relevant constraints such as $\ll H \gg = Tr[H\rho] \equiv U$. Let us maximize

$$S^*[\rho] = -Tr[\rho \ln \rho + \rho\lambda H]$$

where λ is Lagrange multiplier. We set the functional derivative

$\delta S^*/\delta\rho = 0$, which means

$$\lim_{\varepsilon\downarrow 0}\{Tr[(\rho + \varepsilon\eta)\ln(\rho + \varepsilon\eta)] - Tr[\rho \ln \rho] + \lambda Tr[(\rho + \varepsilon\eta)H] - \lambda Tr[\rho\, H\}/\varepsilon = 0 \qquad (22)$$

where $Tr\,\eta = 0$ (i.e. $\rho + \varepsilon\eta$ is a ''nearby'' statistical operator.) Thus by careful inspection of eq. (22), one requires

$$Tr[\eta + \eta(ln\rho + \lambda H)] = Tr[(\ln\rho + \lambda H)\eta] \qquad (23)$$

to be zero for <u>any</u> η that obeys $Tr\,\eta = 0$. Therefore, the rho that achieves this is given by $(\ln\rho + \lambda H) = 0$ or

$$\rho = B\exp(-\lambda H) \equiv \exp(-\lambda H)/Z \qquad (24)$$

where $1/B$ or $Z \equiv Tr[\exp(-\lambda H)]$ is a normalization factor. The Lagrange multiplier λ is $(k\theta)^{-1}$ in usual cases, where θ is the kinetic temperature of the collection of the similar systems. Each collection of systems will have its own in-built meaning of λ, but as it stands in eq. (24) it has dimension of inverse energy.

3. Practical Aspect and Usefulness of Statistical Operator.

As an axiom, there is no isolated material body (except the Universe, of course). Every system has an environment. Let the system have Hamiltonian $H(p,q)$ and its environment$H_e(P,Q)$. The two are coupled, usually nonlinearly so that overall Hamiltonian is

$$H_0(p,P,q,Q) = H_e(P,Q) + H(p,q) + C(q,Q)$$

Since each has at least one degree of freedom, the overall degree of freedom is no less than two, $n \geq 2$. This coupling term $C(q,Q)$ also makes H_0 nonintegrable. It is this coupling that makes analysis so difficult unless one makes the approximation or idealization that C is very weak or nil. Note that the feature of non-integrability is that the sharing of total energy $E = H_0(p,P,q,Q)$ between H_e and H is random, unpredictable and hence chaos.

Quantum mechanically, operator $H(p,q)$ operates on Hilbert space $\mathcal{H}$ and $H_e(P,Q)$ on $\mathcal{H}_e$. The coupled system, with Hamiltonian H_0 operates on direct product space $\mathcal{H}_0 \equiv \mathcal{H}_e \otimes \mathcal{H}$. The overall statistical operator ρ_0 is not necessarily a direct product, $\rho_0 \neq \rho_e \otimes \rho$, in general. However, ρ is the partial trace on $\mathcal{H}_e$ of ρ_0,

$$\rho = Tr_{\mathcal{H}_e}\rho_0 \quad \text{and} \quad \rho_e = Tr_{\mathcal{H}}\rho_0$$

[Think of ρ_0 as a joint probability density $f_0(x,y)$ and ρ_e, ρ as partial probability densities $f_e(y)$, $f(x)$ respectively; $f_e(y) = \int f_0(x,y)dx$, $f(x) = \int f_0(x,y)dy$, $f_0(x,y) \neq f(x)\cdot f_e(y)$].

The expectation value of an observable $A(q,t)$ on $\mathcal{H}$ is given by the density matrix $\rho^{(\mu)}$

$$< A(q,t) >_\psi \equiv < \psi|A|\psi > = Tr\left[A\rho^{(\mu)}\right], \qquad \rho^{(\mu)} \equiv |\psi>< \psi|.$$

But the presence of H_e makes pure density matrix $\rho^{(\mu)}$ inadequate as it influences and makes H to be in several states $|\psi>_*$'s, so that instead of pure $\rho^{(\mu)}$ we have mixed ρ. The statistical averaging

$$\ll A \gg \equiv Tr[A\rho], \qquad \rho \equiv \sum_\mu f_\mu \rho^{(\mu)}, f_\mu \geq 0, \qquad \sum f_\mu = 1$$

is an averaging over the influence of H_e, the environment. This influence is nill in cases where in spite of H_e, ρ remains pure or H_e and H are uncoupled and therefore H isolated. In simple cases like the one that we shall use as an example, H and H_e are harmonic oscillators coupled together nonlinearly.

We should also note the proposition (Ruelle 1969),

$$Tr[\rho_0 \ln\rho_0] \geq Tr[\rho\ln\rho] + Tr[\rho_e \ln\rho_e].$$

Defining entropy $S[\rho\,] \equiv -kTr[\rho\ln\rho]$, we have

$$S_0 \leq S + S_e.$$

5. Quantum Statistical Analysis of Chaotic Hamiltonian : Nonlinearly Coupled Oscillators.

What is the quantum signature of a Hamiltonian system which is classically chaotic? A system has a <u>complete</u> set of observables, at least in principle if it is integrable. For instance, the well-known hydrogenic atom which has <u>three</u> n <u>degrees</u> of freedom has three ν constants of motion, $(\nu = n)$

$$H|\psi> = E|\psi>;\ L^2|\psi> = l(\ell+1)\hbar^2|\psi>;\ L_3|\psi> = m_\ell\hbar|\psi>.$$

It is therefore integrable, like many a quantum system we see in text books.

If $\nu < n$, and H is not explicit in time t then by eq. (24) statistical operator

$$\rho = \rho(H),\ \ H = \text{constant}, E$$

even though system is <u>not</u> integrable.

We consider two identical linear oscillators, each of frequency ω, nonlinearly coupled,

$$2H_0 = p_1^2 + \omega^2 q_1^2 + p_2^2 + \omega^2 q_2^2 + Cq_1^2 q_2^2 \qquad (25)$$

known to be classically chaotic, as we examine its Poincare Section $PS\{q_1 = 0,\ p_1 \geq 0\}$, $C \in \mathbb{R}$ being the coupling constant. On $PS(q_1 = 0,\ p_1 \geq 0)$,

$$\rho = B'\exp(-\lambda\,H) = B'\sum_{p_1>0} exp - \frac{\lambda}{2}(p_1^2 + p_2^2 + \omega^2 q_2^2)) \qquad (26)$$

Let $f(p_1)$ be the fraction of systems that are in quantum state defined by $(q_2\,, p_2)$, with $\sum_{p_{1\geq 0}} f(p_1) = 1$ and

$$B'\sum_{p_{1\geq 0}} f(p_1)\exp(-\lambda p_1^2/2) = B,$$

so that

$$\rho = B\ exp(-\lambda(p_2^2 + \omega^2 q_2^2)/2) \qquad (25')$$

Let $\frac{1}{2}p_2^2 = \frac{-\hbar^2}{2}\ d^2/dx^2$; $\frac{1}{2}\omega^2 q_2^2 \equiv \frac{1}{2}\omega^2 x^2$

The observable

$$W = (-\hbar^2 d^2/dx^2 + \omega^2 x^2)/2$$

has eigenfunctions $\{He_m(x)\exp(-x^2/2)\} \equiv \{\varphi_m(x)\}$ where $He_m(x)$ is Hermite polynomial of degree m

$$He_m(x) \equiv \sum_{r=0}^{m} b_r x^r$$

and with eigenvalues $(m + \frac{1}{2})\hbar\omega$ (cf Merzbacher, 1970).

One easily shows that

$$\ll p_2 \gg = Tr[-i\hbar\ d/dx \exp(-\lambda W)]$$
$$= 0 = \ll q_2 \gg \qquad (26)$$

by mutual orthogonality among $\{\varphi_m(x)\}$.

Furthermore,

$$U \equiv \ll W \gg = Tr[W \exp -\lambda W]/Tr\{\exp(-\lambda W)\}$$
$$= \sum_{m=0}^{N} < \varphi_m(x)|[\quad]|\varphi_m(x) > / \sum_{m=0}^{N} < \varphi_m|\{\quad\}|\varphi_m >$$

where N is finite since $|q_2| \equiv |x| < \infty$. Thus

$$U = \sum_m \left(m + \frac{1}{2}\right)\hbar\omega \exp\left(-\lambda\left(m + \frac{1}{2}\right)\hbar\omega\right) / \sum_m \exp\left(-\lambda\left(m + \frac{1}{2}\right)\hbar\omega\right) \qquad (27)$$

Define

$$Z = \sum_{m=0}^{N} exp\left(-\lambda\left(m + \frac{1}{2}\right)\hbar\omega\right)$$
$$= \exp(-\lambda\hbar\omega/2) \cdot [1 - \exp(-\lambda\hbar\omega(N+1))]/[1 - \exp(-\lambda\hbar\omega)]$$

Let $\alpha \equiv \lambda\hbar\omega$.

$$Z = \exp(-\alpha/2) \cdot [1 - \exp(-(N+1)\alpha]/[1 - \exp(-\alpha)] \qquad (28)$$

$$U = -\frac{\alpha}{\lambda}\frac{d}{d\alpha}\ln Z$$
$$= \frac{\alpha}{\lambda}\{\tfrac{1}{2} - [(N+1)\exp(-(N+1)\alpha)]/[1 - \exp(-(N+1)\alpha)]$$
$$+ \exp(-\alpha)/[1 - \exp(-\alpha)]\}$$
$$= \frac{\alpha}{\lambda}\{\tfrac{1}{2} - (N+1)/[\exp((N+1)\alpha) - 1] + 1/[\exp(\alpha) - 1]\}$$
$$= \hbar\omega\{\tfrac{1}{2} - (N+1)/[\exp((N+1)\alpha) - 1] + [\exp(\alpha) - 1]^{-1}\} \qquad (29)$$
$$\lim_{\hbar\downarrow 0} U = (0 - 0 + 1)/\lambda = \lambda^{-1} \qquad (29')$$

This is as expected classically for a linear oscillator, by the principle of partition of energy (assuming $\lambda = (k\theta)^{-1}$, ϑ being the kinetic temperature)..

With $\rho \equiv \exp(-\lambda H)/Z$, entropy is

$$\ll -ln\rho \gg = -Tr\rho ln\rho = Tr[(\lambda H) + lnZ)\rho]$$
$$= Tr[(\lambda H + lnZ)\exp(-\lambda H)/Z]$$
$$= \lambda U + lnZ \equiv S/k.$$

$$\frac{S}{k} = \alpha\left\{\frac{1}{2} - (N+1)[\exp((N+1)\alpha) - 1]^{-1} + [\exp(\alpha) - 1]^{-1}\right\} + -\frac{\alpha}{2}$$
$$+\ln[1 - \exp(-(N+1)\alpha] - \ln[1 - \exp(-\alpha)]$$
$$= -(N+1)\alpha[\exp((N+1)\alpha - 1]^{-1} + \alpha[\exp(\alpha) - 1]^{-1}$$
$$\ln[1 - \exp(-(N+1)\alpha)] - \ln[1 - exp(-\alpha)] \qquad (30)$$

$$\lim_{\alpha\downarrow 0}\frac{S}{k} = -1 + 1 + \ln(N+1) = \ln(N+1), \qquad N = 0, 1, 2, \ldots \qquad (30')$$

as expected by principle of equiprobability of states.

In the foregoing the effect of coupling C is not obvious. Let us tease out its effect by considering Poincaré section ($q_1 > 0$, $p_1 = 0$)

$H = p_2^2/2 + \Omega^2 q_2^2/2$, $\Omega^2 \equiv (Cq_1^2 + \omega^2)$

$$\rho = \sum_{q_1} \exp(-\lambda H) \equiv Tr\mathcal{H}_1\rho_0$$

On $PS(q_1 = 0,\ p_1 > 0$ we have

$$(-\hbar^2/2m\ \ d^2/dq_1^2 + 0)\,\psi(q_1) = \ \varepsilon\psi(q_1), \quad \varepsilon = \hbar^2k^2/2 > \ 0.$$

(Note, $q_1 = 0 \nRightarrow d/dq_1\ = 0$).

where the energy in the second dof is $E - \varepsilon \le E,\ E$ being the total energy of whole system. On $PS(q_1 \ge 0,\ p_1 = 0$ we have

$$(-\hbar^2/2\ \omega^2\ \ d^2/dq_1^2 + 0)\,\phi(p) = \ \varepsilon\phi(p), \quad \varepsilon = \hbar^2\gamma^2\omega^2/2 > \ 0.$$

In this case,

$$\rho = \sum_{q_1 \ge 0} \exp\,(-\lambda\omega^2 q_1^2/2)\ exp\,(-\lambda W_2)$$

where $W_2 = \frac{1}{2}d^2/dx^2 + \Omega^2/2(q^1)x^2,\ \ \Omega^2 = (Cq_1^2 + \omega^2)$.

In the final analysis, in the limit $C \to 0$, we have $\Omega^2 \to w^2$, and the same results as the foregoing.

6. Conclusion and Remarks

For the nonlinearly coupled oscillators

$$H_0 = (p_1^2 + \omega^2 q_1^2)/2\ + (p_2^2 + \omega^2 q_2^2)/2\ \ + Cq_1^2q_2^2/2$$
$$\equiv H_e + H + {}^1/_2\, Cq_1^2q_2^2 = E$$

at Poincaré section $(q_1 = 0,\ p_1 > 0)$ or $(q_1 > 0,\ p_1 = 0)$ the von Neumann statistical operator ρ depends on $p_1 > 0$ or $q_1 > 0$, which dependence depicts its mixedness and practically the effect of the environment H_e on H. The features of ρ are a glimpse of quantum effects in a (classically) chaotic Hamiltonian system.

The example used is quite simple but it embodies the basic concepts, at least in a two-degree-of-freedom system; that ρ is not in a pure state even for fixed energy E and at a given Poincaré section.

One of the postulates of quantum mechanics is that the commutator C of two observables and the Poisson Bracket PB of their classical counterparts are related by

$C = i\hbar\ PB$. But the supposition of quantum mechanics that a system has a complete set of mutually commuting observables $\{\hat{F}_j\}$ which obey the commutators

$[\hat{F}_j,\ \hat{F}_k] = i\hbar\{F_l, F_k\}\ \ 0, \quad j,k = 1,2,\ldots,n$

is false in a nonintegrable system. For such, one has incomplete knowledge of its dynamical states and hence one must employ statistical operator to convey the incompleteness (Dicke and Wittke, 1960).

Appendix: H_0 is chaotic

We may show that

$$2H_0\ \equiv (p_1^2 + \omega^2 q_1^2) +\ (p_2^2 + \omega^2 q_2^2) +\ Cq_1^2q_2^2\ , C \in \mathbb{R}$$

is (classically) chaotic by numerically exhibiting its behavior on Poincaré Section $q_1 = 0,\ p_1 > 0$ or on $(q_1 > 0,\ p_1 = 0)$. Or by calculating its Lyapunov Exponent, λ_L. The potential part of $2H_0$ is $2V(q_1, q_2)\ \equiv\ \omega^2(q_1^2{+}q_2^2) + Cq_1^2q_2^2$.

The equilibrium points are given by $\partial V/\partial q_1 = \partial V/\partial q_2 = 0$, i.e. at $P(0,0)$ and at $Q(-\omega^2/C,\ \ -\omega^2/C)$, (Solutions of $\omega^2 + Cq_2^2 =\ \omega^2 + Cq_1^2 = 0$).

The Hessian of V at Q is

$$\bar{V} \equiv\ V_{ij} \equiv \left.\begin{pmatrix} \partial^2 V/\partial q_1\partial q_1 & \partial^2 V/\partial q_1\partial q_2 \\ \partial^2 V/\partial q_2\partial q_1 & \partial^2 V/\partial q_2\partial q_2 \end{pmatrix}\right|_Q = \begin{pmatrix} \omega^2 + Cq_2^2 & 2Cq_2^2 \\ 2Cq_2^2 & \omega^2 + Cq_1^2 \end{pmatrix}$$

The stability matrix A is

$$\begin{pmatrix} 0 & I \\ -\bar{V} & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & r & 0 & 0 \\ r & 0 & 0 & 0 \end{pmatrix}, \qquad r\ \equiv\ 2\omega^2,\quad I = 2\times 2\ \ \text{unit.}$$

A has eigenvalues $\pm i\sqrt{2}\omega,\ \ \pm\sqrt{2}\omega$. The largest positive real is $\sqrt{2}\omega$, which is the Lyapunov Exponent λ_L. That is, the separation of two nearby trajectories in time is $\delta(t) = \delta(0)\exp(\sqrt{2}\omega)\,(t)$. $\lambda_L =\ \lim_{t\to\infty}\frac{\ln\,|\delta(t)/\delta(0)|}{t} = \sqrt{2}\omega\ \ \in\ \mathbb{R}_+$

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