Recurrence and coarse-graining in quantum dynamics

1986 J. Phys. A: Math. Gen. 19 L237

(http://iopscience.iop.org/0305-4470/19/5/004)

J. Phys. A: Math. Gen. 19 (1986) L237–L239. Printed in Great Britain

LETTER TO THE EDITOR

Recurrence and coarse-graining in quantum dynamics

Abraham Lozada and P L Torres

Dpto de Física, Facultad de Ciencias, UCV, AP 21201, Caracas 1020-A, Venezuela

Received 21 October 1985, in final form 16 December 1985

Abstract. We consider a microscopic quantum finite dynamical system from which a macroscopic description is obtained. We show that the mean values of observables corresponding to macroscopic states (states obtained from an operation known as a coarse-graining) are almost periodic functions of time.

The recurrence problem for microscopic quantum systems has been considered in the literature emphasising the recurrence of *states* (pure and mixed) with respect to certain topologies (see Bocchieri and Loinger 1957, Percival 1961). In this letter, we consider the problem of the recurrence for *mean values* of observables in finite quantum statistical systems. For other considerations on the recurrence problem for microscopic quantum systems, see, e.g., Hogg and Huberman (1982), Peres (1982) and Lozada and Torres (1984).

A fundamental aim in statistical mechanics is to characterise the (contracted, self-contained) macroscopic description of physical systems from their microscopic behaviour. This characterisation can be accomplished by an operation called coarse-graining (see, e.g., Van Kampen 1962, Emch 1964, 1966, Sewell 1968).

We wish to show in this letter that with the usual coarse-graining operations the recurrence still remains. That is, we show that the mean value of any relevant observable for a macroscopic state (obtained from a coarse-graining operation performed on a microscopic state) is an almost periodic function of time. Recurrence for mean values is what is important physically since all that we can measure in a laboratory are precisely mean values.

We define $\mathcal{T} \subset \mathcal{H} \subset \mathcal{B}$, where $\mathcal{B}$ is the set of all bounded linear operators (with norm $\|\cdot\|$, identity I and X^* standing for the adjoint operator of $X \in \mathcal{B}$) in a separable complex Hilbert space of dimension greater than one, $\mathcal{H}$ is Liouville space (i.e. the space of Hilbert–Schmidt operators, with scalar product $(A, B)_2 \equiv \mathrm{Tr}\, A^*B$, and associated norm $\|\cdot\|_2$) and $\mathcal{T}$ is the set of trace class operators. The observables are all the self-adjoint elements of $\mathcal{B}$, and the set of states ($\mathcal{S}$) is the set of all density operators (i.e. all positive elements, ρ, of $\mathcal{T}$ with $\mathrm{Tr}\,\rho = 1$). We consider a time evolution $A_t \equiv \alpha(t)A \equiv U_t A U_t^{-1}$, $\forall\ A \in \mathcal{H}$, where $u_t = \mathrm{e}^{-\mathrm{i}Ht}$, H being the Hamiltonian (of the closed quantum finite system), such that $\mathrm{Tr}\,\mathrm{e}^{-H} < \infty$.

In a previous article (Lozada and Torres 1984) we proved that the mean values of any observable with any density operator for closed quantum finite dynamical systems is an almost periodic function of time. We now give a brief indication of how this result was obtained. First we show that the function $t \to A_t$ for $A \in \mathcal{H}$ is almost periodic in $\|\cdot\|_2$ (the same proof as in Percival (1961), since elements of $\mathcal{T}$ are used). Then with the inequality

$$|\mathrm{Tr}(\rho_t-\rho)X|\leq 2\|X\|\ \|(\sqrt{\rho})_t-\sqrt{\rho}\|_2 \qquad \forall\rho\in\mathscr{S},\ \forall X\in\mathscr{B} \tag{1}$$

we obtain that the function $t\to\mathrm{Tr}\ \rho_t X$ is almost periodic (since $(\sqrt{\rho})_t\in\mathscr{H}$). The inequality (1) can be proved in the following way:

$$\begin{aligned}|\mathrm{Tr}(\rho_t-\rho)X| &= |\mathrm{Tr}(\sqrt{\rho_t}-\sqrt{\rho})\sqrt{\rho_t}X+\mathrm{Tr}\sqrt{\rho}(\sqrt{\rho_t}-\sqrt{\rho})X|\\ &\leq |(\sqrt{\rho_t}-\sqrt{\rho},\sqrt{\rho_t}X)_2|+|(\sqrt{\rho}X^*,\sqrt{\rho_t}-\sqrt{\rho})_2|\\ &\leq \|\sqrt{\rho_t}-\sqrt{\rho}\|_2(\|\sqrt{\rho_t}X\|_2+\|\sqrt{\rho}X^*\|_2)\\ &\leq \|\sqrt{\rho_t}-\sqrt{\rho}\|_2(\|\sqrt{\rho_t}\|_2+\|\sqrt{\rho}\|_2)\|X\|\\ &= 2\|X\|\ \|\sqrt{\rho_t}-\sqrt{\rho}\|_2\end{aligned}$$

where the well known relations

$$\|AX\|_2\leq\|A\|_2\|X\| \qquad \forall A\in\mathscr{H} \qquad \forall X\in\mathscr{B}$$

and

$$\|X^*\|=\|X\|$$

have been used.

Let $\{D(a)\}\subset\mathscr{B}$ be a set of finite-dimensional projectors, orthogonal to each other, with $\Sigma_a D(a)=I$. We will call the operator $\mathscr{D}:\mathscr{B}\to\mathscr{B}$, given by

$$\mathscr{D}(X)=\sum_a\frac{\mathrm{Tr}(D(a)X)}{W(a)}D(a) \qquad W(a)\equiv\mathrm{Tr}D(a) \qquad X\in\mathscr{B} \tag{2}$$

the *Emch coarse-graining projector* (Emch 1964). We know (Emch 1964) that $\mathscr{D}$ is an orthogonal projection in $\mathscr{H}$, and that it is physically relevant in order to obtain master equations in statistical mechanics (see, e.g., Emch 1964, 1966, Sewell 1968). It is easy to show in a mathematically rigorous way (and trivial to check formally) that

$$\mathrm{Tr}\mathscr{D}(A)X=\mathrm{Tr}\ A\mathscr{D}(X) \qquad \forall A\in\mathscr{T} \qquad \forall X\in\mathscr{B}. \tag{3}$$

With (3) and the quoted result (Lozada and Torres 1984), we conclude that with any coarse-grained state $\sigma_t\equiv\mathscr{D}(\rho_t)$, where $\rho\in\mathscr{S}$ is any density operator, the expectation value of any observable $X\in\mathscr{B}$ (i.e. $\mathrm{Tr}\ \sigma_t X$) will be an almost periodic function of time. We wish to point out that this result is not obvious since the time evolution of σ_t is different from the $\alpha(t)$ one.

Now, guided by the literature in classical generalised equations (see, e.g., Nakajima 1958, Zwanzig 1960, 1961, Mori 1965, Nordholm and Zwanzig 1975, García-Colin and del Río 1977, 1979, Penrose 1979) we see that we can define the following general coarse-graining operation. Let $\mathscr{U}\subset\mathscr{B}$ be any set of fixed observables (they are the physically relevant observables for the problem at hand), and let $\mathscr{P}$ be a time-independent function $\mathscr{P}:\mathscr{S}\to\mathscr{S}$ (not necessarily linear). We will term $\mathscr{P}$ a *coarse-graining operation* (with respect to the set $\mathscr{U}$) if there exists a function $\tilde{\mathscr{P}}:\mathscr{U}\to\mathscr{B}$, such that

$$\mathrm{Tr}\ \mathscr{P}(\rho)X=\mathrm{Tr}\ \rho\tilde{\mathscr{P}}(X) \qquad \forall\rho\in\mathscr{S} \qquad \forall X\in\mathscr{U}. \tag{4}$$

We have (see, e.g., the references quoted immediately above) that this definition is of greater generality than that usually chosen (in fact, in most cases $\tilde{\mathscr{P}}(X)=\mathscr{P}(X)=X$, $\forall X\in\mathscr{U}$; or $\mathscr{U}\subset\mathscr{H}$ and $\mathscr{P}$ is an orthogonal projector in $\mathscr{H}$, in which case (4) holds automatically), and that the Emch coarse-graining projection is a special case thereof (with $\tilde{\mathscr{P}} = \mathscr{P} \equiv \mathscr{D}$; and $\mathscr{U}$ equal to all self-adjoint elements of $\mathscr{B}$). By the same reasoning as above, we obtain that with any coarse-grained state $\sigma_t \equiv \mathscr{P}(\rho_t)$ where $\rho \in \mathscr{S}$ is any density operator, the expectation value of any relevant observable $X \in \mathscr{U}$(i.e. Tr $\sigma_t X$) will be an almost periodic function of time. (We see, once again, that even after a coarse-graining operation is performed, an approach to equilibrium is not obtained; a way out of this difficulty is to take the thermodynamic limit.)

It is also interesting to observe (from (1), (4) and the definition of near-periodicity) that if K is any fixed positive constant, then $\forall \varepsilon > 0$ there exists a $\tau \equiv \tau(\varepsilon)$, common to all observables $X \in \mathscr{U}$, with $\|\tilde{\mathscr{P}}(X)\| < K$, such that for any t

$$|\mathrm{Tr}[\mathscr{P}(\rho_{t+\tau}) - \mathscr{P}(\rho_t)]X| \leq \varepsilon \tag{5}$$

i.e. for a given initial microscopic state ρ the mean values of the coarse-grained state $\mathscr{P}(\rho_t)$ for all relevant observables K in $\mathscr{U}$ with $\|\tilde{\mathscr{P}}(X)\| \leq K$ will recur at the *same* time τ (if the set $\mathscr{U}$ is finite—an often-required condition; K can always be chosen in order that (5) holds $\forall X \in \mathscr{U}$).

If, furthermore, for a coarse-graining operation $\mathscr{P}$, there exist two constants (that depend on the state $\rho \in \mathscr{S}$), α, $M \in (0, \infty)$, such that

$$\|\mathscr{P}(\rho_t) - \mathscr{P}(\rho_{t'})\|_2 \leq M\|\rho_t - \rho_{t'}\|_2^\alpha \qquad \forall t, t' \tag{6}$$

the coarse-grained state $\mathscr{P}(\rho_t)$ will be an almost periodic function of time in $\|\cdot\|_2$ (since ρ_t is an almost periodic function of time in $\|\cdot\|_2$ (Percival 1961)) and in $\|\cdot\|$, because $\|\cdot\| \leq \|\cdot\|_2$. This result is physically less relevant than the near-periodicity for mean values. If $\mathscr{P}$ is any orthogonal projection in $\mathscr{H}$, (6) is automatically satisfied for $M = \alpha = 1$.

References

Bocchieri P and Loinger A 1957 *Phys. Rev.* **2** 337
Emch G G 1964 *Helv. Phys. Acta* **37** 532
—— 1966 *Lectures in Theoretical Physics VIII* ed W E Brittin (Boulder: University of Colorado Press) p 65
García-Colín L S and del Río J L 1977 *J. Stat. Phys.* **16** 235
—— 1979 *Physica* **96A** 606
Hogg T and Huberman B A 1982 *Phys. Rev. Lett.* **48** 711
Lozada A and Torres P L 1984 *Acta Científica Venezolana* **35** 35
Mori H 1965 *Prog. Theor. Phys.* **33** 423
Nakajima S 1958 *Prog. Theor. Phys.* **20** 948
Nordholm S and Zwanzig R 1975 *J. Stat. Phys.* **13** 347
Penrose O 1979 *Rep. Prog. Phys.* **42** 1937
Percival I C 1961 *J. Math. Phys.* **2** 235
Peres A 1982 *Phys. Rev. Lett.* **49** 1118
Sewell G L 1968 *Lectures in Theoretical Physics X-A* ed A O Barut and W E Brittin (New York: Gordon and Breach) p 289
Van Kampen 1962 *Fundamental Problems in Statistical Mechanics* ed E G D Cohen (Amsterdam: North-Holland) p 173
Zwanzig R W 1960 *J. Chem. Phys.* **33** 1338
—— 1961 *Phys. Rev.* **124** 983