On classical and quantal Kolmogorov entropies

J William Helton† and M Tabor‡

† Department of Mathematics, University of California, San Diego, La Jolla, CA 92093, USA
‡ Department of Applied Physics and Nuclear Engineering, Columbia University, New York, NY 10027, USA

Abstract. The construction of a quantal Kolmogorov entropy that tends to the classical Kolmogorov entropy in the limit $\hbar \to 0$ is discussed. The approach is to use sets of functions rather than disjoint partitions and involves the use of pseudo-differential operators.

1. Introduction

The much studied phenomenon of deterministic chaos in Hamiltonian systems has led to some interesting questions concerning the possible implications that this behaviour might have for quantum mechanics in the limit of $\hbar \to 0$.

The *integrable* Hamiltonian systems of classical mechanics form an exceptional but important set of systems. Here, for a system of N degrees of freedom all trajectories are confined to N-dimensional tori embedded in the $(2N-1)$-dimensional energy shell (here we are referring to a conservative Hamiltonian $H = E$). For all initial conditions the system evolves in a highly regular, multiply periodic manner. By contrast, generic Hamiltonians are *non-integrable*. Now the phase space has a most complicated structure of stable and unstable orbits pathologically intertwined. Some trajectories are still confined to tori whereas others wander over large portions of the energy shell in a highly chaotic but entirely deterministic manner. Typically, as nonlinearities in the potential are increased the chaos becomes more and more widespread although it is unlikely that the system becomes ergodic over the *entire* energy shell. (This is certainly true for systems with smooth bounded potentials but certain other systems, such as billiard problems, can be rigorously proven to be ergodic and do, in fact, exhibit even stronger statistical properties [1].)

It was suggested by Percival [2] that there might be a correspondence, in the semiclassical limit $\hbar \to 0$, between quantum mechanics and classical chaos. He termed this regime the 'irregular spectrum' in contrast to the 'regular spectrum' corresponding to the well known correspondence between quantum and classical mechanics in regimes of integrable motion. This idea has led to a variety of interesting investigations (recently revived by Berry [3]). Furthermore there has also been interest in the more general notion of 'quantum chaos'. The meaning and definition of such a concept has proved to be a lively issue.

Work in this direction has tended to fall into two main categories. These are (a) definitions involving a definite *correspondence* in the limit $\hbar \to 0$ between the quantal and classical behaviours and (b) quantum mechanical *analogies* with the classical behaviour. Although one would naturally hope that (b) would also show a correct

classical correspondence in the limit $\hbar \to 0$ this does not necessarily occur. That the two categories should have more than a semantic difference is not surprising since the former definitions require a semiclassical description which is built on a 'skeleton' of classical mechanics whereas the latter definitions are based on purely quantal considerations. The distinction between (a) and (b) has also been made by Kay [4] who carefully defines semiclassical notions of such statistical behaviour as ergodicity and mixing.

An interesting illustration of a quantal definition of a statistical quantity not having the correct classical limit (a feature that by no means invalidates its usefulness) has been in the context of quantal Kolmogorov entropies. In one case, a definition proposed by Kosloff and Rice [5] results in a K-entropy that, for bounded systems, is zero independent of the classical mechanics. (For integrable motion the classical K-entropy is zero and for chaotic motion it is greater than zero.) On the other hand a definition due to Pechukas [6] is non-zero independent of the classical mechanics.

In this paper we propose a definition of a quantal K-entropy that has the correct classical limit. The approach uses sets of functions rather than disjoint partitions and involves the use of pseudo-differential operators. A number of substantial problems arise which we have not been able to fully resolve and it is hoped that this paper will stimulate interest in them. The motivation for this work was provided by other work of the authors on the classical support of quantum mechanical wavefunctions and density matrices [7]. Those results provide a useful background to this paper and are summarised in the next section.

2. The classical support of wavefunctions and density matrices

For integrable systems one may effect the well known canonical transformation to action-angle variables, i.e. $H(p, q) \to H(I)$, where the actions I are constant conjugate momenta. Furthermore the actions are adiabatic invariants and can be quantised according to the Einstein–Brillouin–Keller–Maslov [2] rules where each action is set equal to an integral multiple of $\hbar$ plus a Maslov index (α) i.e.,

$$I = (m + \tfrac{1}{4}\alpha)\hbar, \qquad \text{where } \begin{array}{l} I = I^{(1)}, \ldots, I^{(N)} \\ m = m^{(1)}, \ldots, m^{(N)} \\ \alpha = \alpha^{(1)}, \ldots, \alpha^{(N)}. \end{array} \tag{2.1}$$

Thus the eigenfunction ψ_m has the eigenvalue

$$E_m = H(I) = H((m + \tfrac{1}{4}\alpha)\hbar). \tag{2.2}$$

It is important to note that while for a *fixed* value of $\hbar$ we can associate each eigenstate with a particular classical manifold (the torus defined by (2.1)), as we take the limit $\hbar \to 0$ there will be a whole sequence of states associated with that manifold.

For regimes of strongly chaotic motion no direct semiclassical quantisation procedure has yet been devised. Nonetheless it would be useful to know the nature of the classical support for sequences of states in this regime. Here the authors have proved the following theorem [7].

Theorem. If any sequence of eigenstates of a Hamiltonian H localises to a region R in phase space, then there must be a measure μ supported in R which is invariant under the flow of H.

The way in which one tests eigenfunctions for localisation in phase space is non-trivial and involves the use of pseudo-differential operators (some of the basic properties of these are summarised in the appendix). It is then a standard result of functional analysis to show that

$$L\{(\hat{O}_f \psi_{k_l}, \psi_{k_l})\} = \int f_m \, d\mu \tag{2.3}$$

where L denotes a Banach limit [8] (which could, e.g., for simple cases just be the limit $l \to \infty$), μ is a locally bounded Borel measure (supported in R) and f_m is the principal symbol of the (pseudo-differential) operator $\hat{O}_f$. The double subscript on the eigenfunctions ψ_{k_l} pertains to the usual mathematical convention of talking in terms of subsequences of eigenfunctions (rather than just sequences). The invariance of the measure under the Hamiltonian flow is demonstrated through the use of Egorov's theorem (see appendix). The theorem also holds for families of density matrices $\{\rho_l\}$, i.e.,

$$L\{\mathrm{Tr}(\hat{O}_f \rho_l)\} = \int f_m \, d\mu \tag{2.4}$$

where again μ is an invariant measure supported on some closed set R in phase space. Thus the above results demonstrate the way in which operators and families of density matrices can be associated, in the limit $\hbar \to 0$ (i.e. through the use of the Banach limit (2.4)), with classical functions (the principal symbols) and invariant measures (the μ).

3. Classical and quantal entropies

We first of all construct the standard K-entropy for the classical case. For completeness we include some standard background [1]. If $P = \{P_1, \ldots, P_k\}$ is a partition of the manifold R, then the entropy of P is

$$H(P) = -\sum_{i=1}^{k} \mu(P_i) \ln \mu(P_i). \tag{3.1}$$

The entropy of some transformation T relative to P is

$$H(T, P) = \lim_{n \to \infty} \frac{1}{n} H\left(\bigvee_{i=1}^{n} T^i P\right) \tag{3.2}$$

where $\bigvee_{i=1}^{n} T^i P$ represents the join $P \vee TP \vee \ldots \vee T^n P$. In terms of the measure we can thus write

$$H(T, P) = -\lim_{n \to \infty} \frac{1}{n} \sum_{i_1, i_2, \ldots, i_n} \mu(P_{i_1} \cap TP_{i_2} \cap \ldots \cap T^n P_{i_n}) \ln \mu(P_{i_1} \cap \ldots \cap T^n P_{i_n}). \tag{3.3}$$

It is a standard result to show that the entropy $H(T, P)$ can be expressed as

$$H(T, P) = \lim_{n \to \infty} H\left(P \,\middle|\, \bigvee_{i=1}^{n} T^{-i} P\right)$$

where $H(P | \bigvee_{i=1}^{n} T^{-i} P)$ represents the conditional entropy of P given $\bigvee_{i=1}^{n} T^{-i} P$. What this implies is that if the partition P can be inferred from the previous n partitions (which would correspond to a quasiperiodic evolution) then $H(T, P)$ is zero. The

K-entropy $H(T)$ is defined as the supremum of $H(T, P)$ over all partitions P, i.e.,

$$H(T) = \sup_P H(T, P). \tag{3.4}$$

This supremum can be shown to be finite for a fairly wide class of (classical) transformations [1].

Before we proceed to the quantal case we introduce the notion of characteristic functions. For the partition P we may associate a function χ_i with each atom P_i. If the 'phase point' lies in P_i then $\chi_i = 1$; otherwise $\chi_i = 0$. Now consider the partitions P at different times t_l and t_m. Then we have

$$\chi_i(t_l)\chi_j(t_m) = \delta_{ij}\chi_j \qquad \text{if } t_l = t_m \tag{3.5a}$$

$$= \chi(P_i(t_l) \cap P_j(t_m)) \qquad \text{if } t_l \neq t_m \tag{3.5b}$$

where $\chi(P_i(t_l) \cap P_j(t_m)) = 1$ if the phase point lies in the intersection $P_i(t_l) \cap P_j(t_m)$; otherwise $\chi = 0$. Then, by definition, it follows that

$$\int \chi_i(t_l)\chi_j(t_m)\, d\mu = \int \chi(P_i(t_l) \cap P_j(t_m))\, d\mu$$

$$= \mu(P_i(t_l) \cap P_j(t_m)). \tag{3.6}$$

In order to construct a quantal version of the K-entropy one might be tempted to proceed directly to a quantum mechanical analogue of the classical phase space partition. A natural choice here would be to take sets of orthogonal projection operators $\hat{P}_j$ satisfying $\hat{P}_j\hat{P}_k = \delta_{jk}\hat{P}_j$ and $\sum_{j=1}^m \hat{P}_j = 1$ (cf (3.5a)). This is the starting point used by both Kosloff and Rice [5] and Pechukas [6]. However, the latter author goes on to show that there are certain subtleties in the measurement process which leads to his formulation having a different end result to that of the former authors.

Here we take a different route which, subject to certain technicalities, should lead to the correct classical limit. In order to make the transition to a quantal description we must first smooth the χ_j (which behave like step functions) into differentiable functions b_j such that the b_j are 'within ε' of the χ_j. Thus, whereas the χ_j admit the orthogonality property

$$(1 - \chi_j)\chi_j = 0 \tag{3.7}$$

(cf (3.5a)), we allow the b_j to behave as

$$(1 - b_j)b_j = O(\varepsilon). \tag{3.8}$$

Additional constraints on condition (3.8) will be discussed later. The family of functions $\ell = \{b_1 \ldots b_k\}$, which might be termed an 'ε-disjoint partition' can be constructed to satisfy the condition

$$b_j \geq 0, \qquad \sum_{j=1}^k b_j = 1 \tag{3.9}$$

i.e., they constitute a partition of unity. Using the notation

$$b_i(k\tau) = b_i \circ g_{k\tau},$$

where the right-hand side denotes composition with the (Hamiltonian) flow g_t over k

equal time periods τ, we define the integral

$$I(g_t; \ell) = \int b_{i_1}(\tau) b_{i_2}(2\tau) \ldots b_{i_n}(n\tau) \, d\mu. \tag{3.10}$$

Using (3.6) we can thus define the 'ε-entropy' of g_t relative to ℓ

$$H_\varepsilon(g_t; \ell) = -\lim_{n\to\infty} \frac{1}{n} \sum_{i_1\ldots i_n} I(g_t; \ell) \ln I(g_t; \ell) \tag{3.11}$$

and hence the corresponding K-entropy as

$$H_\varepsilon(g_t) = \sup_\ell H_\varepsilon(g_t; \ell). \tag{3.12}$$

A crucial technical point, whose relevance to the quantal problem will soon become apparent, is the fate of the supremum after taking the limit $\varepsilon \to 0$. Naturally we would hope that

$$\lim_{\varepsilon\to 0} H_\varepsilon(g_t) = H(g_t). \tag{3.13}$$

Clearly this will depend on the behaviour of the ℓ_j's in this limit. Additional constraints over and above (3.8) may be required such as

$$\sum_{j=1}^{k} (1 - b_j) b_j < \delta \tag{3.14}$$

or even for example,

$$\int dx (1 - b_j) b_j \log[(1 - b_j) b_j] < \delta. \tag{3.15}$$

(The authors would like to thank Michael Aizenman and Joel Lebowitz for suggesting constraints of the form (3.14) and (3.15).) Not only must we consider the limit $\varepsilon \to 0$ (3.13) but we must also consider the possibility of the supremum taken in (3.12) being bounded by a minimum partition 'size'—in this case the phase volume of a quantum state h^N. However this seems unlikely to destroy the boundedness of the supremum. Clearly a rigorous resolution of the technicalities raised here would be most valuable. Some aspects have been touched on by Brin and Katok [9].

The quantal description is effected by using the family of functions $\ell = \{b_1, \ldots, b_k\}$ as the principal symbols for a family of pseudo-differential operators $\mathcal{B} = \{B_1, \ldots, B_k\}$. The B_j's are taken to satisfy the conditions

$$B_j > 0, \qquad \sum_{j=1}^{k} B_j = 1. \tag{3.16}$$

Since ℓ is an ε-disjoint partition the B_j cannot be taken to be strictly orthogonal. We now associate with any density matrix ρ and evolution operator U the quantal analogue of the integral (3.10), i.e.,

$$Q(U; \mathcal{B}, \rho_t) = \text{Tr}(B_{i_1} U B_{i_2} U \ldots U B_{i_n} \rho_t) \tag{3.17}$$

where $U = \exp(it\sqrt{H})$. The use of $\sqrt{H}$ rather than H in the evolution operator is in keeping with Egorov's theorem on the evolution of pseudo-differential operators under Hamiltonian flows (see appendix). (In (3.17) we use the fact that $U^{-i}U^{i+1} = U$.)

The entropy of U relative to $\mathscr{B}$ is thus just

$$H^{(\text{Quant})}(U; \mathscr{B}) = \lim_{n \to \infty} \frac{1}{n} \sum_{i_1 \dots i_n} Q(U; \mathscr{B}, \rho) \ln Q(U: \mathscr{B}, \rho) \tag{3.18}$$

and the corresponding K-entropy is then

$$H^{(\text{Quant})}(U) = \sup_{\mathscr{B}} H^{(\text{Quant})}(U; \mathscr{B}). \tag{3.19}$$

Another interesting technical question arises that again concerns the supremum. The operators B_j have only been defined up to their principal symbols b_j. It is quite possible that there could exist compact perturbations (C_j) to the B_j that are sufficiently badly behaved to wreck the supremum in (3.19). One can hope that the conditions (3.16) will mitigate this problem [10]. If not, it would be nice to find a systematic procedure for further restricting the admissible C_j to obtain the desired behaviour.

We remark that our definition of $H^{(\text{Quant})}(U; \mathscr{B})$ looks not dissimilar to that proposed by Pechukas [6], although in that work, as in [5], the observables are not taken to be pseudo-differential but a strictly orthogonal projection. In view of our results it might be worth examining this assumption more closely. The key seems to be less in the form of (3.17) than in the class of observables one admits.

The final stage is to show the connection, in the limit $\hbar \to 0$, between the classical (3.11), (3.12) and quantal (3.18), (3.19) entropies. Suppose $\{\rho_l\}$ is a sequence of density matrices for which (2.4) holds for some Banach limit L. Then (cf § 2)

$$L\{Q(U; \mathscr{B}, \rho_l)\} = I(g_t; \ell). \tag{3.20}$$

This formally makes it appear that the quantum entropy for the ρ_l's approaches the classical entropy for μ.

To recapitulate there are two problems: the most serious is the interchange of $\sup(\mathscr{B})$ with $\lim(l \to \infty)$ in (3.19) and (3.20). Only if the entropy is invariant under this interchange can we rigorously say that the quantal entropy approaches the classical entropy H_ε. The other problem concerns whether $\lim_{\varepsilon \to 0} H_\varepsilon = H$; this question might not be too hard to resolve, although for our semiclassical model the 'smoothness' ε may itself have to be $\hbar$ dependent—this would then make the limits particularly delicate.

Appendix

Here we summarise just a few of the basic properties of pseudo-differential operators [11]. Consider some well behaved test function $u(x)$ in $\mathbb{R}^n$ with the usual Fourier

transform and inverse, i.e.,

$$\tilde{u}(\xi) = \frac{1}{(2\pi)^{n/2}} \int_{\mathbf{R}^n} e^{-ix\xi} u(x) \, dx$$

$$u(x) = \frac{1}{(2\pi)^{n/2}} \int_{\mathbf{R}^n} e^{ix\xi} \tilde{u}(\xi) \, d\xi. \tag{A1}$$

The effect of some (differential) operator $\hat{O}_f$ operating on u can then be represented as

$$\hat{O}_f u(q) = \frac{1}{(2\pi)^n} \int_{\mathbf{R}^n} \int_{\mathbf{R}^n} \exp[i(q-q')\xi] f(q, \xi) u(q') \, dq' \, d\xi \tag{A2}$$

where the polynomial (in ξ) $f(q, \xi)$ is called the full symbol of the operator $\hat{O}_f$. It can be decomposed into a sum of homogeneous terms

$$f(q, \xi) = f_m(q, \xi) + f_{m-1}(q, \xi) + \ldots f_j \ldots \tag{A3}$$

with f_j homogeneous in ξ of degree j. The leading term f_m is called the principal symbol of $\hat{O}_f$. Pseudo-differential operators are operators defined as above but the f are not longer restricted to be polynomials in ξ. However the f_j are still required to be homogeneous in ξ, i.e., the symbol f has the asymptotic expansion

$$f(q, \xi) \simeq \sum_{n=-\infty}^{|m|} f_n(q, \xi), \qquad |\xi| \to \infty \tag{A4}$$

where the f_n's are homogeneous in ξ.

The pseudo-differential character of $\hat{O}$ is preserved under Hamiltonian flow providing the square root of the Hamiltonian is used, i.e.,

$$\hat{O}_{f_t} = e^{i\sqrt{H}t} \hat{O}_f \, e^{-i\sqrt{H}t}. \tag{A5}$$

Egorov's theorem states that

$$f_m(t) = f_m \circ g_t \tag{A6}$$

where the right-hand side of (A6) represents composition of the principal symbol f_m with the flow g_t (i.e., $f \circ g(t) = f(q(t), (t))$). As is easily demonstrated the flow under $\sqrt{H}$ is the same as that under H subject to a rescaling of time. In general (A5) is not exact and corrections arise at lower order (than the principal symbol). For our purposes, however, these corrections will disappear when the Banach limit (2.3) is taken.

References

[1] Arnol'd V I and Avez A 1968 *Ergodic Properties of Classical Mechanics* (New York: Benjamin)
[2] Percival I C 1977 *Adv. Chem. Phys.* **36** 1
[3] Berry M V 1981 *Semiclassical Mechanics of Regular and Irregular Motion, Les Houches Lecture Notes* ed G Iooss, R H G Helleman and R Stora (Amsterdam: North-Holland)
[4] Kay K G 1983 *J. Chem. Phys* **79** 3026
[5] Kosloff R and Rice S A 1980 *J. Chem. Phys.* **72** 1337
[6] Pechukas P 1982 *J. Phys. Chem.* **86** 2239
[7] Helton J W and Tabor M 1985 *Physica* **14D** 409-15
[8] Royden H L 1968 *Real Analysis* 2nd edn (New York: McMillan)
[9] Brin M and Katok A 1981 in *Geometric Dynamics (Proc. Conf. Rio de Janeiro (1981) Lecture Notes 1007)* ed J Palis Jr (Berlin: Springer)
[10] Ehrenfreud G Private communication
[11] Nirenberg L 1972 *Lectures on Partial Differential Equations (Conf. Board of Math. Sci. No 17)* (Providence, RI: Am Math. Soc.)