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# A comparison of exact and semiclassical analysis of diagonal occupation probabilities for the Feingold–Peres chaotic Hamiltonian

E R Pike†‡, Sarben Sarkar‡ and J S Satchell‡

† Department of Physics, King's College, London WC2R 2LS, UK

‡ Centre for Theoretical Studies, Royal Signals and Radar Establishment, Great Malvern, Worcestershire WR14 3PS, UK

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**Abstract.** A semiclassical analysis is given for general chaotic Hamiltonians of the short-time quantum dynamics of survival probabilities of pure initial states in canonical bases. This is illustrated for the Feingold-Peres coupled spin model which is classically chaotic. The dynamics predicted by the semiclassical arguments is compared with exact quantum mechanics and is found to be remarkably accurate even for $\hbar$ as large as 0.23.

Much of the progress in the understanding of quantum systems, which classically show chaos, has been in terms of the properties of the distribution of adjacent energy level spacings [1] and other statistics such as the spectral rigidity [2]. These properties are found to fall into a small set of universality classes. There is no such overall understanding of dynamics. In this paper we will consider certain dynamical calculations for general chaotic Hamiltonians. These concern the time dependence of the occupation probability of an initial non-stationary pure state. This problem has attracted attention previously [3] but the considerations have been heuristic and relied on numerical experiments [3-5] which were qualitatively interpreted as due to non-stationary initial states having 'ergodic' or 'democratic' overlaps with the energy eigenstates of the system. For any quantum system with a small number of participating states in the dynamics, sizeable recurrences will appear and the correspondence with any classical features will be difficult to disentangle. It is expected that in the semiclassical limit such correspondences will emerge. In the context of lowest-order semiclassical analysis we will be able to be more precise about 'ergodic' overlaps. Our analysis leads to quantitative predictions and the enunciation of a 'democracy principle' for quantised chaotic systems which agree well with numerical experiments on moderately small quantum systems for the coupled spin model [4, 6].

Occupation probabilities are diagonal density matrix elements. If $\rho$ is the density matrix and $H$ is the Hamiltonian, then the Schrödinger equation implies that

$$\rho(t) = \exp\left(-\frac{\mathrm{i}Ht}{\hbar}\right)\rho(0)\exp\left(\frac{\mathrm{i}Ht}{\hbar}\right). \tag{1}$$

For any complete set of states $\{|m\rangle;\ m = 0, 1, 2, \ldots\}$ and set of energy eigenstates $\{|N\rangle;\ N = 0, 1, 2, \ldots\}$ we have

$$\rho_{jk}(t) = \sum_{N,M} \exp\left(-\frac{\mathrm{i}}{\hbar}(E_N - E_M)t\right)\rho'^{jk}_{NM} \tag{2}$$

where

$$\rho^{jk}_{NM} = \sum_{n,m} C^{(j)}_N C^{(n)*}_N C^{(m)}_M C^{(k)*}_M \rho_{nm}(0) \tag{3}$$

$$\rho_{jk}(t) = \langle j|\rho(t)|k\rangle \tag{4}$$

$$H|N\rangle = E_N|N\rangle \tag{5}$$

and

$$C^{(q)}_p = \langle q|P\rangle. \tag{6}$$

Although the above is quite general our semiclassical analysis requires further restrictions. In particular we consider

$$\rho_{nm}(0) = \delta_{nn_0}\delta_{mn_0} \tag{7}$$

and states $|m\rangle$ which are eigenstates of either $\hat{\boldsymbol{p}}$ or $\hat{\boldsymbol{q}}$, the canonically conjugate momenta and coordinates, respectively.

A minimal requirement on a chaotic system is that it is ergodic. Berry [7] and Voros [8] were influenced by this requirement and postulated that the Wigner function $W(\boldsymbol{p}, \boldsymbol{q})$ corresponding to a chaotic eigenstate of energy $E$ is given by the measure appropriate to a microcanonical ensemble, i.e.

$$W(\boldsymbol{p}, \boldsymbol{q}, E) = \frac{\delta(H(\boldsymbol{p}, \boldsymbol{q}) - E)}{\iint \mathrm{d}^D p\, \mathrm{d}^D q\, \delta(H(\boldsymbol{p}, \boldsymbol{q}) - E)} \tag{8}$$

where $D$ is the number of degrees of freedom of the system and $\boldsymbol{p}$ and $\boldsymbol{q}$ are canonically conjugate $c$-number momenta and coordinates. Knowing the Wigner function allows us to calculate semiclassically

$$|C^{(m)}_N|^2 = \iint \mathrm{d}^D p\, \mathrm{d}^D q\, \delta(m - n(\boldsymbol{p}, \boldsymbol{q}))\, W(\boldsymbol{p}, \boldsymbol{q}, E_N) \tag{9}$$

where $n(\boldsymbol{p}, \boldsymbol{q})$ is either $\boldsymbol{p}$ or $\boldsymbol{q}$ depending on the choice of the basis set $\{|m\rangle\}$. For systems with closely spaced energy levels it is useful to introduce a coarse-graining scale $\Delta E$ and write (2) as

$$\sum_{N,M} \rho^{jk}_{NM} \exp\left(-\mathrm{i}(E_N - E_M)\frac{t}{\hbar}\right) \simeq \sum_E \exp\left(-\frac{\mathrm{i}Et}{\hbar}\right) \sum_{\substack{N,M \\ E \leqslant E_N - E_M < E + \Delta E}} \rho^{jk}_{NM}. \tag{10}$$

From now on we will exclusively consider the calculation of $\rho_{n_0 n_0}(t)$:

$$\rho_{n_0 n_0}(t) = \sum_E (\Delta E)\tilde{\rho}_{n_0 n_0}(E) \exp\left(-\frac{\mathrm{i}Et}{\hbar}\right) + \mathrm{O}((\Delta E)^2) \tag{11}$$

where we define

$$\tilde{\rho}_{n_0 n_0}(E) = \sum_{\substack{N,M \\ E \leqslant E_N - E_M < E + \Delta E}} |C^{(n_0)}_N||C^{(n_0)}_M|^2/\Delta E. \tag{12}$$

It is straightforward to show that

$$\tilde{\rho}_{n_0 n_0}(E) = \int \mathrm{d}E'\, \tilde{\psi}(E')\tilde{\psi}(E' + E) \tag{13}$$

where

$$\tilde{\psi}_m(E_N) = |C_N^{(m)}|^2 \Omega(E_N) \tag{14}$$

and

$$\Omega(E) = \iint \mathrm{d}^D p\, \mathrm{d}^D q\, \delta(E - H(\boldsymbol{p}, \boldsymbol{q})) \tag{15}$$

is the single-sided density of states. Classically an ergodic system democratically visits all parts of phase space in the sense of a time average. Quantum mechanically $\tilde{\psi}_m(E_N)$ is the probability of overlap of an initial state with the state space of energy eigenstates where the integration measure is the democratic one of $\mathrm{d}E$. We expect that $\tilde{\psi}_m(E_N)$ will be largely structureless (except possibly near special symmetry points of the Hamiltonian) and thus reflect the democratic principle in the quantum chaotic case.

In the limit $\Delta E \to 0$, (11) gives the simple Fourier transform relationship

$$\rho_{n_0 n_0}(t) = \int_{-\infty}^{\infty} \tilde{\rho}_{n_0 n_0}(E) \exp\left(-\frac{\mathrm{i}Et}{\hbar}\right) \mathrm{d}E. \tag{16}$$

Equations (9) and (13)-(16) summarise the theoretical development. The value of this approach will be illustrated within the context of an autonomous spin Hamiltonian. An advantage of spin models is that the quantum theory involves only the dynamics of finite-dimensional matrices and so can be handled exactly. Feingold and Peres have introduced an interesting continuous time non-integrable model [4, 6] which consists of two coupled spins. The total angular momentum of each spin is separately conserved. We recall briefly the details of the model. The Hamiltonian is

$$H = H_0 + V$$

with

$$H_0 = L_3 + M_3 \tag{17}$$

and

$$V = L_1 M_1 . \tag{18}$$

The angular momenta $L_i$ and $M_i$ $(i = 1, 2, 3)$ satisfy the algebra

$$\begin{aligned} [L_i, Lj] &= \mathrm{i}\varepsilon_{ijk}\hbar L_k \\ [M_i, M_j] &= \mathrm{i}\varepsilon_{ijk}\hbar M_k \\ [L_i, M_j] &= 0. \end{aligned} \tag{19}$$

A natural representation of the basis of quantum states is in terms of the direct product of standard angular momentum states $|l, m\rangle|l, m'\rangle$. For simplicity we take $L = M$ where $L^2 = l(l+1)\hbar^2$. The action of the operators $L_i$ on $|l, m\rangle$ is

$$\begin{aligned} L_3|l, m\rangle &= m\hbar|l, m\rangle \\ (L_1 \pm \mathrm{i}L_2)|l, m\rangle &= [l(l+1) - m(m \pm 1)]^{1/2}\hbar|l, m \pm 1\rangle \end{aligned} \tag{20}$$

where $-l \leqslant m \leqslant l$. Similar relations hold for the operators $M_i$ when acting on the states $|l, m'\rangle$.

Classically the motion in phase space is predominantly regular for $L<1$ and $L>4$. From numerical work [6] it is known that $L=3.5$ gives chaos for a large interval of energy values. For this $L$, in our direct numerical analysis of the model, we will take $l=14.5$ and this gives $\hbar \sim 0.23$. This is the largest value of $l$ that we can conveniently use. From such computations it will emerge that the semiclassical theory is remarkably useful for calculating $\rho_{n_0 n_0}(t)$ even for systems with such large $\hbar$.

For the coupled spin model the semiclassical analysis for $\tilde{\psi}(E)$ (cf (9), (14) and (15)) gives

$$\tilde{\psi}^{(l_3,m_3)}(E)=\int \mathrm{d}^2q \int \mathrm{d}^2p\,\delta(p_1-l_3)\delta(p_2-m_3)$$
$$\times\,\delta[E-p_1-p_2-(L^2-p_1^2)^{1/2}(L^2-p_2^2)^{1/2}\cos q_1\cos q_2] \qquad (21)$$

where

$$L_1=(L^2-p_1^2)^{1/2}\cos q_1$$
$$L_2=(L^2-p_1^2)^{1/2}\sin q_1 \qquad (22)$$
$$L_3=p_1.$$

Identical relations with $(p_1, q_1)$ replaced by $(p_2, q_2)$ give expressions for $M_i$ $(i=1,2,3)$. The variables $(p_j, q_j)$ $(j=1,2)$ are just the canonically conjugate momenta and coordinates for the coupled spin model. The integrals in (21) can be evaluated to give (for $E<2l$)

$$\tilde{\psi}^{(l_3,m_3)}(E)=\frac{4\theta[(L^2-l_3^2)(L^2-m_3^2)-(E-l_3-m_3)^2]}{[(L^2-l_3^2)(L^2-m_3^2)]^{1/2}}F(\pi/2,\sin(q_2)_0) \qquad (23)$$

where

$$\theta(x)=\begin{cases}1 & \text{for} \quad x>0\\ 0 & \text{otherwise}\end{cases}$$

$$(q_2)_0=\cos^{-1}\left(\frac{E-l_3-m_3}{(L^2-l_3^2)^{1/2}(L^2-m_3^2)^{1/2}}\right)$$

(with $0\leqslant(q_2)_0\leqslant\pi$) and

$$F(\varphi,k)=\int_0^{\varphi}\frac{\mathrm{d}y}{(1-k^2\sin^2 y)^{1/2}}.$$

Moreover

$$\Omega(E)=\int_{-\pi}^{\pi}\mathrm{d}q_2\frac{1}{\cos q_2}\left[\sin^{-1}\left(\frac{(p_2)_1\cos q_2}{(1+L^2\cos^2 q_2)^{1/2}}\right)-\sin^{-1}\left(\frac{L\cos q_2}{(1+L^2\cos^2 q_2)^{1/2}}\right)\right] \qquad (24)$$

where in the integrand

$$(P_2)_1=\frac{E-L[-E^2\cos^2 q_2+(1+l^2\cos^2 q_2)^2]^{1/2}}{1+L^2\cos^2 q_2}.$$

These formulae can, even in principle, only be valid approximately since there is always some small regular part of phase space. However, as we shall see, they are rather accurate. The relevant integrals need to be done numerically.

Figures 1-4 summarise the ability of our semiclassical analysis to describe the dynamics of the coupled spin model with $L=3.5$. The semiclassical prediction of

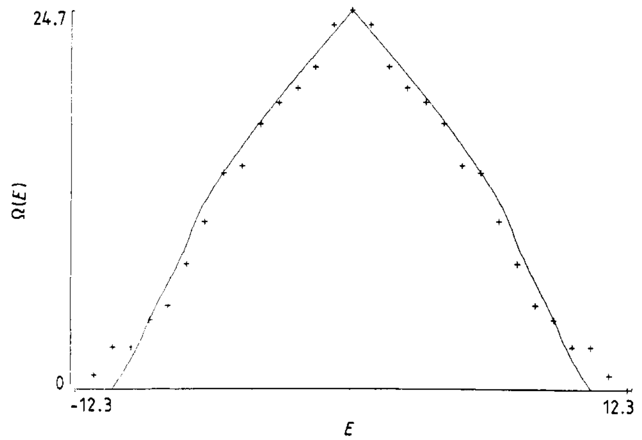


**Figure 1.** $\Omega(E)$ for semiclassical (−) and $\hbar=0.23$ (+) calculations.

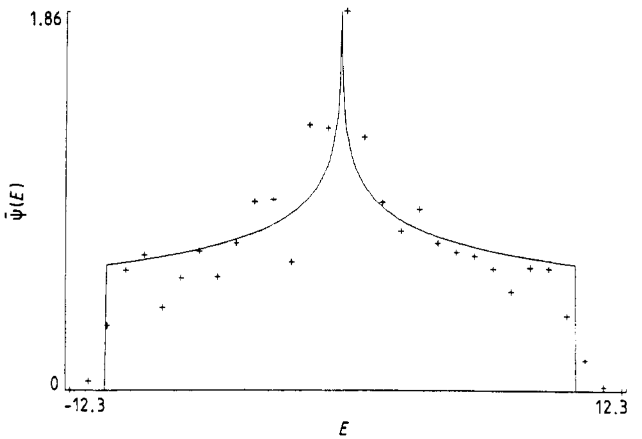


**Figure 2.** $\tilde{\psi}(E)$ for semiclassical (--) and $\hbar=0.23$ (+) calculations.

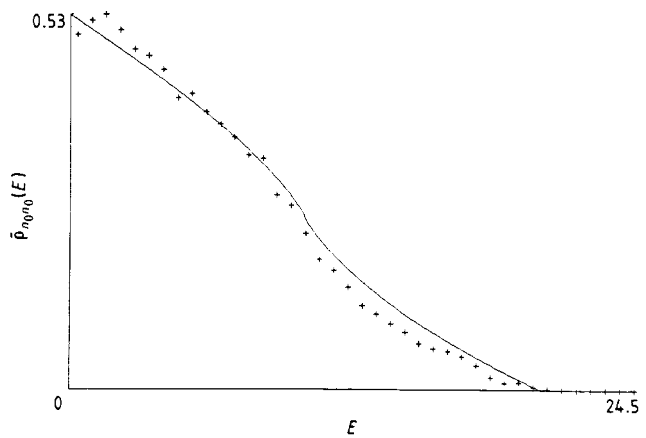


**Figure 3.** $\tilde{\rho}_{n_0n_0}(E)$ for semiclassical (−) and $\hbar=0.23$ (+) calculations.

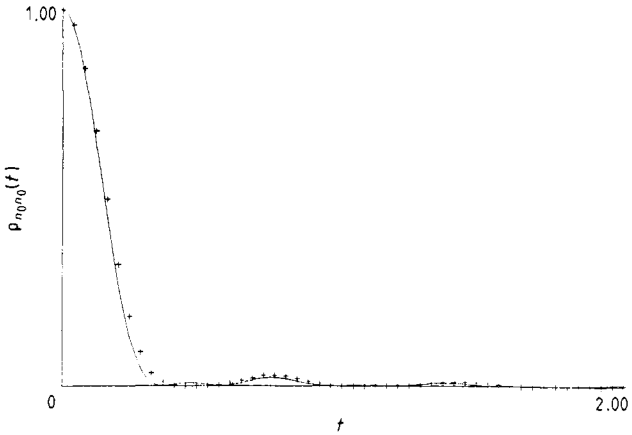


**Figure 4.** $\rho_{n_0n_0}(t)$ for semiclassical (−) and $\hbar = 0.23$ (+) calculations.

$\Omega(E)$ is only valid for the range of $E$ where chaotic behaviour is predominant. (In fact, earlier numerical investigations showed that phase space was mainly chaotic for $|E| < 6.6$ and mainly regular for $|E| > 9.9$.) Consequently the value of $\Omega(E)$ falls to zero prematurely at values of $E$ which correspond to the purely regular regions of the model. For smaller values of $E$ the qualitative agreement between the semiclassical and full quantum results is very good as can be seen in figure 1. $\tilde{\psi}(E)$ also shows good agreement between the semiclassical and fully quantum results for an initial state with $L_3 = 1.28$ and $M_3 = -1.52$. It is true that the statistics are not good. However, the important features of the restriction of $\tilde{\psi}(E)$ to the energy shell (i.e. the constraint of the $\theta$ function) and a peak at $E = L_3 + M_3$ are found. The quantity $\tilde{\rho}_{n_0n_0}(E)$ is of crucial importance to the dynamics; it shows truly impressive agreement between finite $\hbar$ and semiclassical calculations. As a result the behaviour of $\rho_{n_0n_0}(t)$ predicted by the semiclassical analysis agrees very well with the full quantum calculation with

$$\hbar \sim 0.23.$$

In conclusion we have shown explicitly that semiclassical analysis can be used to describe quite accurately the decay of pure initial states for a Hamiltonian which classically shows chaos. This description will be valid for times of the order of the inverse of the coarse-graining scale. Semiclassically this is a large time. The techniques that we have used to calculate the dynamics should apply equally well to chaotic Hamiltonians.

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## References

[1] Casati G (ed) 1985 *Chaotic Behavior in Quantum Systems* (New York: Plenum)
Pike E R and Lugiato L A (ed) 1987 *Chaos, Noise and Fractals* (Bristol: Adam Hilger)

Pike E R and Sarkar S (ed) 1987 *Quantum Measurement and Chaos* (New York: Plenum)
[2] Berry M V 1985 *Proc. R. Soc.* A **400** 229
[3] Heller E J and Sundberg R L 1985 *Chaotic Behavior in Quantum Systems* ed G Casati (New York: Plenum) p 225
[4] Feingold M and Peres A 1985 *Phys. Rev.* A **31** 2472
[5] Pike E R, Sarkar S and Satchell J S 1987 *Quantum Measurement and Chaos* ed E R Pike and S Sarkar (New York: Plenum) p 119
[6] Feingold M and Peres A 1983 *Physica* **9D** 433
[7] Berry M V 1977 *J. Phys. A: Math. Gen.* **10** 2083
[8] Voros A 1979 *Stochastic Behaviour in Classical and Quantum Hamiltonian Systems* (*Lecture Notes in Physics* **93**) ed G Casati and J Ford (Berlin: Springer) p 326