Quantum signatures of chaos in integrable systems

1995 J. Phys. A: Math. Gen. 28 5701

(http://iopscience.iop.org/0305-4470/28/20/004)

J. Phys. A: Math. Gen. 28 (1995) 5701–5708. Printed in the UK

Quantum signatures of chaos in integrable systems

V Constantoudis and N Theodorakopoulos

Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, Vas. Constantinou 48, GR-116 35 Athens, Greece

Received 1 May 1995

Abstract. Two fundamental quantum signatures of classically chaotic behaviour, large second derivatives and the logarithmic time barrier separating classical from quantum dynamics, have been observed near the separatrix of an integrable spin system. A systematic study in the neighbourhood of the separatrix reveals that the error in semiclassical eigenvalues (measured in units of the quantum level spacing) approaches a finite value at the classical limit. The generic factor which limits the validity of the correspondence principle is the presence of classical instabilities; chaotic behaviour is one such case; the separatrix of an integrable system is another.

1. Introduction

Research in chaos, i.e. the area where classical and quantum descriptions of relatively simple physical systems appear to be in fundamental conflict, has placed the semiclassical limiting process at a natural focus of interest. This has been especially clear in the dynamics of the crossover from classical to quantum behaviour [1]: systems which are classically chaotic begin to exhibit quantum behaviour after a very short time (logarithmically divergent as $\hbar \to 0$); systems which are classically non-chaotic take longer to reveal their quantum nature; the crossover time diverges as an inverse power of $\hbar$.

It is well known that the onset of chaos in Hamiltonian systems which exhibit both bounded and unbounded behaviour in phase space, occurs near the separatrix; tori in that neighbourhood are the first to break up according to the KAM scenario. On an apparently unrelated level, it has been observed [2] that the spacing of quantum levels near the classical separatrix in a double-well potential approaches the classical limit very slowly (logarithmically) as $\hbar \to 0$. The authors of [2] characterize this practical limitation of the correspondence principle as a macroscopic quantum effect. Bearing in mind that the 'observable' under consideration in [2] is in fact a frequency, it is natural to regard the difference $\Delta\omega$ between quantum mechanical and classical frequencies as a measure of the distance from the classical limit; the inverse quantity $2\pi/\Delta\omega$ represents the observation time needed to achieve the frequency resolution $\Delta\omega$, i.e. it quantifies the validity of classical dynamics in the time domain.

Taken together, the results of [1,2] suggest that the same logarithmic divergence which characterizes the relatively fast crossover from classical to quantum behaviour in (classically) chaotic systems appears in a context which is (at first sight) unrelated to chaos. In order to pursue this intriguing question further, we have studied a classically integrable spin system. The system offers some practical advantages in regard to the study of the classical limit. On the one hand, it is possible to perform highly accurate quantum mechanical calculations for large values of the spin S, i.e. 'near' the classical limit. On the other hand, the approach

0305-4470/95/205701+08$19.50

to the classical limit $S \to \infty$ can be followed systematically, according to Fisher's [3] procedure.

We have calculated the error occurring in semiclassical energy eigenvalues (measured in units of the level spacing [4]). This quantity provides a direct measure of the approach to classicality. Our conclusions go beyond those of [4]. Not only does the semiclassical approximation fail to predict individual energy levels near the separatrix, in the sense that the error is bounded from below; even at the limit $S \to \infty$ the error remains finite. Similar conclusions hold for the relative error of the semiclassically computed frequencies. In terms of dynamics, our findings extend those of [2] to spin systems. The logarithmic dependence of $\Delta\omega$ on the classicality parameter gives rise to the same 'macroscopic' quantum effects. Away from the classical separatrix, the correspondence principle exhibits its standard 'robustness'; the errors vanish as power laws of $1/S$.

2. Classical dynamics

We consider the two-spin-S XXZ Hamiltonian

$$H = J(S_1 \cdot S_2 + \Delta S_1^z S_2^z). \tag{2.1}$$

At the classical limit of (2.1), defined by [3,5] $\hbar \to 0, S \to \infty, \hbar S \to S_{cl}, J \to 0, J\sqrt{S(S+1)} \to j$, the spin operators can be substituted by unit vectors $\{\sigma_i\}$. We employ a system of dimensionless variables, in which energies and times are measured in units of j and S_{cl}/j, respectively. Furthermore, we use canonical variables [6] defined by $p_i = \sigma_i^z, \tan\phi_i = \sigma_i^y/\sigma_i^x$.

A further reduction is possible by exploiting the rotational invariance of (2.1) with respect to the z-axis. Using the canonical transformation

$$(p_1, p_2, \phi_1, \phi_2) \to (p = p_1, p_T = p_1 + p_2, \phi = \phi_1 - \phi_2, \chi = \phi_2) \tag{2.2}$$

and setting, without loss of generality, $p_T = 0$, we reduce the dynamics to a single degree of freedom, described by the classical Hamiltonian

$$H_{cl}(p, \phi) = (1 - p^2)\cos\phi - (1 + \Delta)p^2. \tag{2.3}$$

Hamilton's equations for (2.3) can be solved exactly in terms of elliptic functions. The topology of trajectories in phase space (figure 1) differs according to the value of the anisotropy parameter. The topology of type I is similar to that of a simple pendulum, whereas the topology of type II has not been found in known particle systems and appears to be a distinct feature of spin dynamics. Both topologies are characterized by the presence of separatrices.

The action variable can be defined on the torus of energy E as

$$I(E) = \frac{1}{2\pi}\oint p\,\mathrm{d}\phi = \frac{1}{2\pi}\oint \sqrt{\frac{\cos\phi - E}{1 + \Delta + \cos\phi}}\,\mathrm{d}\phi. \tag{2.4}$$

It is possible to use action variables defined in a p-representation, i.e. as integrals over $\mathrm{d}p$; such action variables are related to (2.4) via a Legendre transformation.

For tori which are in the neighbourhood of the separatrix, the frequency is given asymptotically by

$$\omega(E) = \frac{\partial E}{\partial I} \sim -\frac{\lambda}{\ln|E - E_{sep}|} \tag{2.5}$$

where E_{sep} is the energy at the separatrix, and λ the instability exponent which characterizes the unstable fixed point contained in the separatrix. The exponent λ expresses the rate

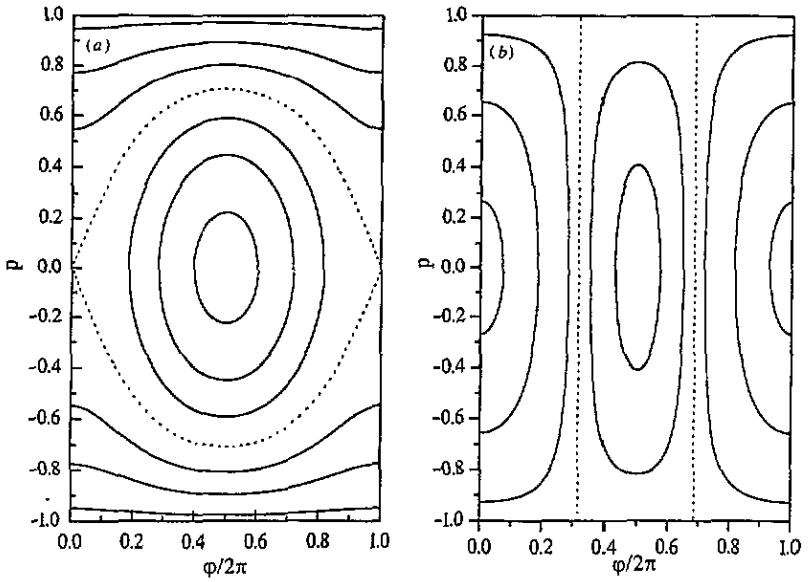

Figure 1. (*a*) Type I topology has one unstable fixed point at $p = 0, \phi = 0$ with $\lambda = \sqrt{-2(2+\Delta)}$ if $\Delta < -2$ or at $p = 0, \phi = \pi$ with $\lambda = \sqrt{2\Delta}$ if $\Delta > 0$. This phase space diagram is drawn for $\Delta = -4$. (*b*) Type II topology occurs for $-2 < \Delta < 0$. There are two unstable fixed points at $p = \pm 1$ with instability exponent $\lambda = \sqrt{-\Delta(2+\Delta)}$. This phase space diagram is drawn for $\Delta = -0.6$.

at which a point belonging to the unstable (stable) manifold of the hyperbolic fixed point recedes from (approaches) the fixed point. In other words, it is a local Lyapounov exponent.

3. Semiclassical quantization

In order to perform the WKB quantization procedure for a spin system, it is first necessary to write down Schrödinger's equation in differential form; to do this, we use Villain's [7] transformation

$$\begin{aligned} S_n^+/\overline{S} &= \mathrm{e}^{\mathrm{i}\hat{\phi}_n}\sqrt{1-\hat{p}_n^2-\frac{\hat{p}_n}{\overline{S}}} \\ S_n^-/\overline{S} &= \sqrt{1-\hat{p}_n^2-\frac{\hat{p}_n}{\overline{S}}}\,\mathrm{e}^{-\mathrm{i}\hat{\phi}_n} \qquad n=1,2 \end{aligned} \tag{3.1}$$

where $\hat{p}_n = S_n^z/\overline{S}$ and $\overline{S} = \sqrt{S(S+1)}$ ($\sim S + \frac{1}{2}$ for large values of S); using (3.1) it is possible to rewrite the quantum Hamiltonian in terms of the canonically conjugate operators $\hat{p} = \hat{p}_1$ and $\hat{\phi} = \hat{\phi}_1 - \hat{\phi}_2$ (again setting $S_{\mathrm{tot}}^z = 0$ without loss of generality) as

$$H_{\mathrm{qu}}(\hat{p},\hat{\phi}) = \frac{1}{2}\left[\sqrt{1-\hat{p}^2-\frac{\hat{p}}{\overline{S}}}\,\mathrm{e}^{\mathrm{i}\hat{\phi}}\sqrt{1-\hat{p}^2+\frac{\hat{p}}{\overline{S}}}+\mathrm{HC}\right]-(1+\Delta)\hat{p}^2\,. \tag{3.2}$$

Schrödinger's equation in the p-representation follows from (3.2) by the substitution $\hat{\phi} = -\frac{1}{\overline{S}}\frac{\mathrm{d}}{\mathrm{d}p}$. The WKB method can now be formulated as in particle systems. The

quantization rules follow from the demand that the semiclassical wavefunction should be single-valued. They are slightly dependent on the type of torus considered:

$$I(E_n) = \frac{n + \frac{1}{2}}{S + \frac{1}{2}} \qquad \text{(oscillational tori, } n \text{ any positive integer)} \tag{3.3}$$

and

$$I(E_n) = \frac{\frac{1}{2}n}{S + \frac{1}{2}} \qquad \text{(degenerate rotational tori (type I topology only), } \Delta n = 2). \tag{3.4}$$

The Hamiltonian (2.1) is tridiagonal in the subspace corresponding to $S^z_{\text{tot}} = 0$ and can be readily diagonalized to give the quantum mechanical spectrum. As a test of the numerical procedure, we have checked for the presence of pairs of eigenvalues which are exactly symmetric around zero for $\Delta = -1$ (any S). The pairs sum to values of $\mathcal{O}(10^{-15})$ for $S = 1000$ and $\mathcal{O}(10^{-14})$ for $S = 5000$.

In the type I topology, quantum eigenvalues which correspond to rotational tori appear almost degenerate due to dynamical tunnelling [8, 9]. The quantization conditions (3.4) must be supplemented by the tunnelling splitting. The semiclassical spectrum computed by numerical solution of (3.3) and (3.4) is in good agreement with the exact one, except in the neighbourhood of E_{sep}; in this case, it is possible to improve on the WKB procedure following Miller's method, originally developed for potential tunnelling [10]; semiclassical spectra near E_{sep}, computed according to [10], represent a substantial improvement compared to those obtained by the standard WKB method; in particular, it is possible to obtain quite good values (i) for the energies of non-degenerate states and (ii) for the tunnelling splitting of degenerate states.

Type II topology is characterized by the absence of (dynamical) tunnelling. The semiclassically computed (non-degenerate) spectrum is in good agreement with the exact one, except in the neighbourhood of E_{sep}.

In order to test the quality of the semiclassical approximation, it is expedient [4] to examine the difference $\Delta E_{\text{s,q}}$ between corresponding semiclassical and quantum eigenvalues, E_{sc} and E_{qu}, respectively, measured in units of the energy level spacing ΔE_{qu} of quantum eigenvalues. A small ratio, compared to unity, is a minimum requirement for a meaningful semiclassical approximation, since it allows a one-to-one correspondence between semiclassical and quantum spectra. A ratio which tends to zero in the classical limit might be expected on general grounds of the correspondence principle. The findings of [4] for the one-dimensional potential $U(x) = U_0/\cos^2(x)$ suggest that the situation is more subtle; in the limit of large quantum numbers the ratio remains finite, bounded by the finiteness of $\hbar$; for a given quantum number, it approaches zero (as $\hbar$) in the limit $\hbar \to 0$. In our case, we are dealing with a system with a finite number of states ($\mathcal{O}(S)$), hence our classical limiting process $\hbar \to 0, S \to \infty, \hbar S \to S_{\text{cl}}$, is necessarily of the second type.

We have computed the ratio

$$\delta\epsilon(E_{\text{sep}}, S) = \frac{\overline{\Delta E}_{\text{s,q}}}{\overline{\Delta E}_{\text{qu}}} \tag{3.5}$$

as a function of S. The averages are taken over the four states closest to the classical separatrix. Results are shown in figure 2; the striking feature is that the dimensionless ratio $\delta\epsilon$ approaches a finite value (0.08) in the limit $S \to \infty$, i.e. the semiclassical approximation fails to predict individual energy levels *even in the limit* $S \to \infty$.

A similar calculation of $\delta\epsilon$ for energies far from E_{sep} shows that the ratio approaches zero as $1/S$. We thus conclude that the presence of the separatrix 'undermines' the validity of the semiclassical approximation.

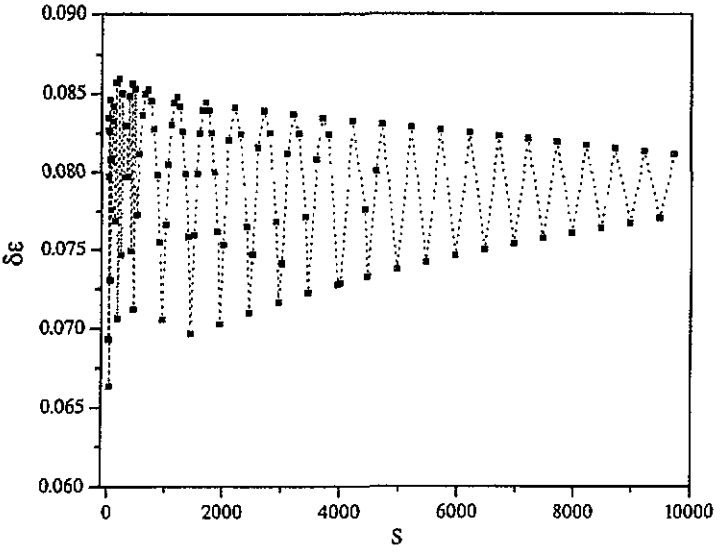

Figure 2. The deviation of the semiclassical energy eigenvalues from the exact quantum eigenvalues divided by the (quantum) level spacing is plotted as a function of S, for $\Delta = -0.6$. Both numerator and denominator represent averages over the four eigenvalues closest to the separatrix energy. The dotted curves are a guide to the eye.

4. Separatrix and the correspondence principle: implications for quantum chaos?

One of the first, and probably one of the most fundamental, formulations of the correspondence principle is that the quantum frequency $\omega_{qu} = (E_{n+1} - E_n)/\hbar$ must, in the limit $\hbar \to 0$, approach the classical frequency of the torus with action $I_n = I(E_n)$ (more exactly, the torus with action $(I_n + I_{n+1})/2$).

We have computed ω_{qu} as a function of S, from the difference of the quantun eigenvalues E_+ and E_- lying immediately above and below the separatrix, respectively. The corresponding classical frequency ω_{cl} is defined as the oscillation frequency on the torus with energy $(E_+ + E_-)/2$ (the torus with action $(I_+ + I_-)/2$ leads to the same results). Results of our calculations, shown in figure 3, reveal a slow (logarithmic) convergence of both quantities to zero. The slow approach of ω_{qu} to 0 (more precisely, of the difference $\delta\omega = \omega_{qu} - \omega_{cl}$, cf below) can be compared with the findings of [2] regarding the appearance of quantum effects in a macroscopic system (particle in a potential well). In order to clarify the influence of the separatrix, we have performed the same calculation away from E_{sep}; in this case the difference between quantum and classical frequencies approaches zero as $1/S^2$ in the limit of large S.

Having established the link of the separatrix to the manifestation of macroscopic quantum effects (or, alternatively, to the limitations of the correspondence principle) the next step is to examine the dependence of $\delta\omega$ on the magnitude of the instability related to the classical separatrix, as expressed by λ. Our results for a number of different values of λ, shown in figure 4, demonstrate that in the limit $S \to \infty$,

$$\delta\omega = A\frac{\lambda}{\ln S} \tag{4.1}$$

where $A \sim \mathcal{O}(1)$. Equation (4.1) can also be interpreted in terms of the 'observation time'

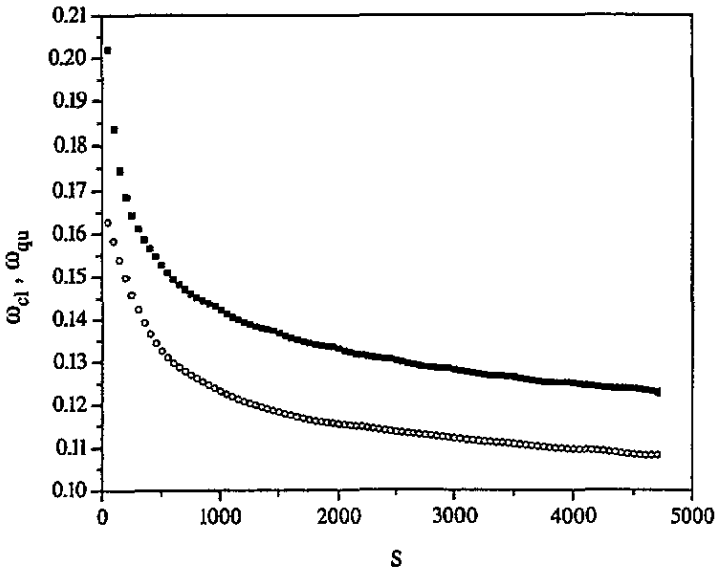

Figure 3. Quantum (full squares) and classical (open circles) frequencies near the separatrix (of the text for exact definitions). Note the slow (logarithmic) decay.

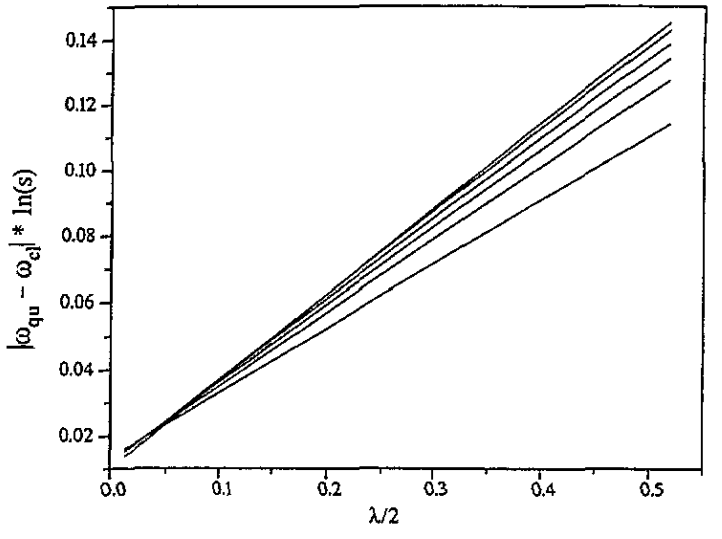

Figure 4. The rescaled frequency difference $(\omega_{qu} - \omega_{cl}) \ln S$ as a function of the instability index. The straight lines are convoluted fittings of our results and correspond, from bottom to top, to $S = 10, 50, 100, 200, 500$ and 1000, respectively. The asymptotic limit is characterized by the inverse logarithmic and linear dependence on S and λ, respectively. The inverse of $\delta\omega$ is the crossover time, known in quantum chaology as the log barrier.

necessary to achieve the 'frequency resolution' $\delta\omega$, i.e. the crossover time

$$t_{cr} \propto \frac{\ln S}{\lambda} \tag{4.2}$$

beyond which a quantum wavepacket does not follow the dynamics of an identical ensemble

of classical orbits.

The logarithmic restriction of the agreement between classical and quantum dynamics is one of the most fundamental quantum signatures of chaos. The crossover time for a classically chaotic system is given by a relationship [1, 11] which is formally identical to (4.2), and in which λ is the Lyapounov exponent of the chaotic motion. This has been explained on the basis of the exponential sensitivity of classical orbits to the initial conditions. Equation (4.2), however, arises in a classically integrable system and can be understood on the basis of the following simple argument:

Consider a minimum uncertainty wavepacket initially centred at the unstable fixed point. In both topologies, its energy width ΔE will be proportional to $1/S$. The rate at which the wavepacket spreads is proportional to the spread in the group velocities of its components—in our case the classical torus frequencies. Hence

$$t_{cr} \propto 1/\omega_{cl} \propto -\frac{\ln \Delta E}{\lambda} \propto \frac{\ln S}{\lambda} . \tag{4.3}$$

The above simple argument demonstrates that the absence of quantum chaos in classically chaotic systems and the macroscopic quantum effects near the separatrix of a classically integrable system are both manifestations of the weakest possible validity of the correspondence principle—the 'logarithmic barrier'; the latter's origins can, in both cases, be traced to (and quantified by the characteristic exponent of) a local instability.

An equally interesting similarity occurs in the behaviour of another suggested diagnostic tool of chaos, namely the large second differences of quantum eigenvalues with respect to a perturbational parameter. Pompfrey [12] confirmed numerically the suggestion made by Percival [13] that large second derivatives of energy eigenvalues are a sign of classically chaotic behaviour. The work of Noid *et al* [14] on Henon–Heiles-like systems showed that such derivatives appear in connection with energies which participate in avoided crossings,

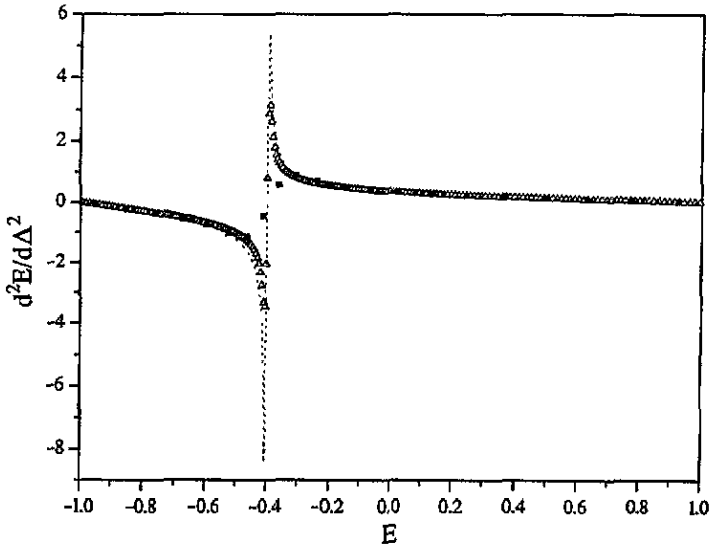

Figure 5. Second derivatives of energy eigenvalues with respect to the anisotropy Δ for $S = 10$ (full squares) and $S = 100$ (open triangles). Also drawn (dotted curve) is the corresponding classical quantity $(\partial^2 E/\partial^2 \Delta)_I$. The large values of second derivatives are known to be a quantum signature of classical chaos. This figure shows that the classical limit of these derivatives also becomes singular at the separatrix of an integrable system.

and suggested that the appearance of a single, isolated avoided crossing is associated with a new resonance (generating a separatrix) in phase space. The above relationships can be established more clearly in a system with a single degree of freedom.

Figure 5 displays the dependence of the second derivative of the eigenvalues of (2.1) with respect to the anisotropy parameter, as a function of the energy, for $S = 10$ and 100. We observe, in agreement with [14], that the second derivative changes sign at $E = E_{sep}$ and grows significantly in the vicinity of E_{sep}. The change in sign is a signature of the avoided crossing. Also plotted in figure 5 is the classical quantity $(\partial^2 E/\partial^2 \Delta)_I$; the derivative taken at constant action allows us to follow the dependence of a given torus' energy on Δ; thus, the quantity plotted represents the classical limit of the quantum mechanical second derivatives. Again, we observe that the basic features of an important diagnostic tool of quantum chaology is already apparent, at the classical level, near the separatrix of an integrable system.

References

[1] Berry M and Bolazs N 1979 *J. Phys. A: Math. Gen.* **12** 625
[2] Cary J R, Rusu P and Skodje R T 1987 *Phys. Rev. Lett.* **58** 4
[3] Fisher M E 1964 *Am. J. Phys.* **32** 343
[4] Prosen T and Robnik M 1992 *J. Phys. A: Math. Gen.* **26** L37
[5] Manson M 1975 *Phys. Rev.* B **12** 400
[6] Magyari E, Thomas H, Weber R, Kaufman C and Müller G 1987 *Z. Phys.* B **65** 363
[7] Villain J 1974 *J. Physique* **35** 27
[8] Davies M and Heller E 1981 *J. Chem. Phys.* **75** 846
[9] Stuckebrukhor A and Marcus R 1993 *J. Chem. Phys.* **98** 8443
[10] Miller W 1968 *J. Chem. Phys.* **48** 1651
[11] D'Ariano G, Evangelista L and Saraceno M 1992 *Phys. Rev.* A **45** 3646
[12] Pompfrey N 1974 *J. Phys. B: At. Mol. Phys.* **7** 1909
[13] Percival J 1977 *Adv. Chem. Phys.* **36** 1
[14] Noid D, Koszykowski M and Marcus R 1983 *J. Chem. Phys.* **78** 4018