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Level Density of the Hénon-Heiles System Above the Critical Barrier Energy

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Abstract. We discuss the coarse-grained level density of the Hénon-Heiles system above the barrier energy, where the system is nearly chaotic. We use periodic orbit theory to approximate its oscillating part semiclassically via Gutzwiller's semiclassical trace formula (extended by uniform approximations for the contributions of bifurcating orbits). Including only a few stable and unstable orbits, we reproduce the quantum-mechanical density of states very accurately. We also present a perturbative calculation of the stabilities of two infinite series of orbits (R_n and L_m), emanating from the shortest librating straight-line orbit (A) in a bifurcation cascade just below the barrier, which at the barrier have two common asymptotic Lyapunov exponents χ_{R} and χ_{L}.

The two-dimensional Hénon-Heiles (HH) Hamiltonian

$$H_{HH} = T + V_{HH}(x,y) = \frac{1}{2}\,(p_x^2 + p_y^2) + \frac{1}{2}\,(x^2 + y^2) + \alpha\,(x^2 y - y^3/3) \qquad (1)$$

was introduced [1] to describe the mean gravitational field of a stellar galaxy. It describes an open system in which a particle can escape over one of three barriers with critical energy $E_{bar} = 1/6\alpha^2$ and has meanwhile become a textbook example [2, 3, 4] of a system with mixed dynamics reaching from integrable motion (for $E \to 0$) to nearly fully chaotic motion (for $E \gtrsim E_{bar}$). Scaling coordinates and momenta with α causes the classical dynamics to depend only on the scaled energy $e = E/E_{bar} = 6\alpha^2 E$; the barrier energy then lies at $e = 1$.

The Hamiltonian (1) has also been used [5] to describe the nonlinear normal modes of triatomic molecules, such as H_3^+, whose equilibrium configuration has D_3 symmetry. Although this model may no longer be quantitative for large energies, it can qualitatively describe the dissociation of the molecule for $e > 1$.

In this paper we discuss the coarse-grained level density of the HH Hamiltonian (1) above the barriers, calculated both quantum-mechanically and semiclassically using periodic orbit theory. Since the potential V_{HH} in (1) goes asymptotically to $-\infty$ like $-r^3$ ($r^2 = x^2 + y^2$) in some regions of space, the quantum

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spectrum of (1) is strictly speaking continuous. However, for sufficiently small α there are quasi-bound states for $E < E_{bar}$ whose widths are exponentially small except very near E_{bar}. For semiclassical calculations of the HH level density for $e < 1$, we refer to earlier papers [6, 7]. In [8] we have calculated the complex resonance energies $E_m - i\Gamma_m$ by the standard method of complex rotation, diagonalizing (1) in a finite harmonic-oscillator basis. The level density is, after subtracting the non-resonant part of the continuum, given by

$$\Delta g(E) = -\frac{1}{\pi}\,\mathrm{Im}\sum_m \frac{1}{E - E_m + i\,\Gamma_m/2}\,. \tag{2}$$

We define the *coarse-grained* level density by a Gaussian convolution of (2) over an energy range γ

$$\Delta g_\gamma(E) = \frac{1}{\gamma\sqrt{\pi}}\int_{-\infty}^{\infty}\Delta g(E')\,e^{-(E-E')^2/\gamma^2}\,\mathrm{d}E', \tag{3}$$

which can be done analytically [8]. Its oscillating part, which describes the *gross-shell structure* in the quantum-mechanical level density, is then given by

$$\delta g_{qm}(E) = \Delta g_\gamma(E) - \widetilde{\Delta g}(E), \tag{4}$$

where $\widetilde{\Delta g}(E)$ is the smooth part of (2) which we have extracted by a complex version [8] of the numerical Strutinsky averaging procedure [9].

Semiclassically, the quantity $\delta g(E)$ can be approximated by Gutzwiller's trace formula [10], which for a system with two degrees of freedom reads

$$\delta g_{scl}\,(E) = \frac{1}{\pi\hbar}\sum_{po}\frac{T_{po}(E)}{r_{po}\sqrt{|\mathrm{Tr}\,\mathrm{M}_{po}(E)-2|}}\,e^{-[\gamma T_{po}(E)/2\hbar]^2}\cos\left[\frac{S_{po}(E)}{\hbar}-\frac{\pi}{2}\,\sigma_{po}\right]. \tag{5}$$

The sum goes over all isolated periodic orbits labeled 'po', and the other quantities in (5) are the periods T_{po} and actions S_{po}, the Maslov indices σ_{po} and the repetition numbers r_{po} of the periodic orbits. $\mathrm{M}_{po}(E)$ is the stability matrix obtained by linearization of the equations of motion along each periodic orbit. The Gaussian factor in (5) is the result of a convolution analogous to (3); it suppresses the orbits with long periods and hence yields the gross-shell structure in terms of the shortest periodic orbits, hereby eliminating the convergence problem characteristic of non-integrable systems [3]. This use of the trace formula to describe gross-shell quantum effects semiclassically has found many applications in different fields of physics (including interacting fermion systems in the mean-field approximation; see [4] for examples).

The shortest periodic orbits of the classical HH system (1) have already been extensively studied in earlier papers [11, 12, 13]. In [8] we have calculated all relevant orbits and their properties from the classical equations of motion and computed the quantity $\delta g_{scl}(E)$ in (5). Some of the shortest orbits are shown in the left part of Fig. 1, all evaluated at $e = 1$ (except for τ_2 which is evaluated at $e = 1.1$). Note that due to the D_3 symmetry of the HH potential, the orbits A_5, B_4, τ_2 and L_6 (as well as all orbits R_n and L_m bifurcating from A, see below)

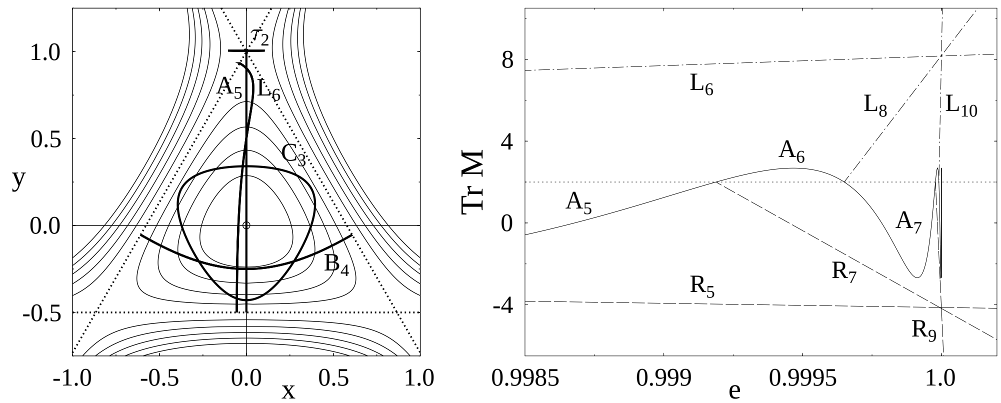

Figure 1. *Left:* Contours of the HH potential and some of its shortest periodic orbits in the (x, y) plane (see text). *Right:* Trace of the stability matrix of the A orbit and the three pairs of orbits (R_5,L_6), (R_7,L_8), (R_9,L_{10}) bifurcated from it, forming the beginnings of the 'HH fans'.

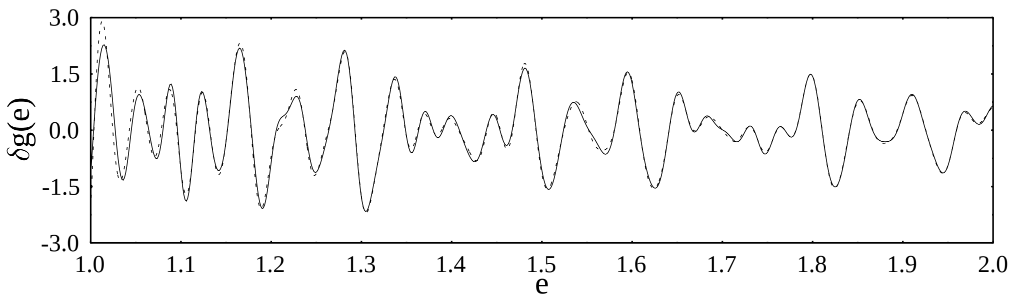

Figure 2. Comparison of quantum-mechanical (solid line) and semiclassical (dashed line) level density $\delta g(E)$ of the HH potential versus scaled energy e, coarse grained with Gaussian smoothing range $\gamma = 0.25$. Only 18 periodic orbits contribute to the semiclassical result [8].

have two symmetry partners obtained by rotations about $\pm 2\pi/3$. The orbit C_3 and all triplets of R_m orbits have a time reversed partner each.[1]

In Fig. 2 we show a comparison of semiclassical (5) with quantum-mechanical (4) results, both coarse-grained with $\gamma = 0.25$ (units such that $\hbar = 1$). At this resolution of the gross-shell structure, only 18 periodic orbits contribute to the semiclassical result; for the period-two orbit D_7 which is stable up to $e \simeq 1.29$ and involves to further orbits (E_8, G_7) in a codimension-two bifurcation scenario, we have used the appropriate uniform approximation [14] to avoid the divergence of the trace formula (5) (see [8] for details). We note that the agreement of semiclassics with quantum mechanics is excellent. Only near $e \sim 1$ there is a slight discrepancy which is mainly due to some uncertainties in the numerical extraction of $\widetilde{\Delta g}(E)$. We can conclude that also in the continuum region above

[1] We use here the nomenclature introduced in [12, 13], where the Maslov indices σ_{po} appear as subscripts of the symbols (B_4, R_5, L_6, etc.) of the orbits.

a threshold, the semiclassical description of quantum shell effects in the level density of a classically chaotic system works quantitatively.

In view of the importance of the level density close to the critical barrier energy $e = 1$ for the threshold behaviour of a reaction described by the HH model potential, we focus now on a particular set of periodic orbits existing at $e = 1$. The straight-line librating orbit A reaches this energy with an infinite period after undergoing an infinite cascade of bifurcations for $e \to 1$. At these bifurcations, two alternating infinite sequences of rotational orbits R_n $(n = 5, 7, 9, \ldots)$ and librating orbits L_m $(m = 6, 8, 10, \ldots)$ are born; their bifurcation energies e_n and e_m form two geometric progressions converging to $e = 1$ with a 'Feigenbaum constant' $\delta = \exp(2\pi/\sqrt{3}) = 37.622367\ldots$; the shapes of these new orbits are self-similar when scaled with $\sqrt{\delta}$ in both x and y direction (see [12] for details). The stability traces of the first three pairs (R_n, L_m) are shown in the right part of Fig. 1. As seen there, the curves $\mathrm{TrM}(e)$ of these orbits are nearly linear (at least up to $e \sim 1.02$) and intersect at $e = 1$ approximately at the same values for each type (R or L). For large n and m, these values were found numerically [12] to be $\mathrm{TrM}_{\mathrm{L}_m}(e = 1) \sim 8.183$ and $\mathrm{TrM}_{\mathrm{R}_n}(e = 1) \sim -4.183$. This means that at $e = 1$, all L orbits have asymptotically the same Lyapunov exponent $\chi_{\mathrm{L}} \simeq 2.087$, and all R orbits have the same Lyapunov exponent $\chi_{\mathrm{R}} \simeq 1.368$. Based upon these numerical findings, we postulate the following asymptotic behaviour:

$$\mathrm{TrM}_{\mathrm{R}_n,\mathrm{L}_m}(e) \;\sim\; 2 \mp 6.183 \left(\frac{e - e^*}{1 - e^*} \right) \qquad \text{for} \qquad e \to 1\,, \quad n, m \to \infty\,. \tag{6}$$

Here e^* are the respective bifurcation energies of the orbits (e_n or e_m), and the minus or plus sign is to be associated with the R or L orbits, respectively. The curves $\mathrm{TrM}_{\mathrm{R}_n,\mathrm{L}_m}(e)$ thus form two 'fans' spreading out from the values 8.183 and -4.183 at $e = 1$, the first three members of each being shown in the right part of Fig. 1. In the following we will sketch briefly how the qualitative features in (6) of these 'HH fans' can be obtained analytically from semiclassical perturbation theory. Details will be given in a forthcoming publication [15].

The idea is to start from the following 'separable HH' (SHH) Hamiltonian

$$H_0 = H_{SHH} = \frac{1}{2}\,(p_x^2 + p_y^2) + \frac{1}{2}\,(x^2 + y^2) - \frac{\alpha}{3}\,y^3 \tag{7}$$

and to include the term $\alpha\, x^2 y$ in first-order perturbation theory. Formally, we multiply it by a small positive number ϵ and write $H_{HH} = H_0 + \epsilon H_1$ with $H_1 = \alpha\, x^2 y = u^2 v/\alpha^2$, where $u = \alpha x$ and $v = \alpha y$ are the scaled coordinates. The Hamiltonian (7) is integrable; an analytical trace formula for it has been given in [7]. There is only one saddle at $(x, y) = (0, 1)$ with energy $e = 1$ and one librating A orbit along the y axis which undergoes an infinite cascade of bifurcations for $e \to 1$. From it, an infinite sequence of rational tori T_{lk} bifurcates, where l is their repetition number and $k = 2, 3, \ldots$ counts the bifurcations (and the tori). The v motion of the primitive A orbit ($l = 1$), having $u_A(t) = 0$, is given by

$$v_A(t) = v_1 + (v_2 - v_1)\,\mathrm{sn}^2(at, q)\,, \quad a = \sqrt{\frac{v_3 - v_1}{6}}\,, \quad q = \sqrt{\frac{v_2 - v_1}{v_3 - v_1}} \tag{8}$$

in terms of the Jacobi elliptic function [16] $\mathrm{sn}(z,q)$ with modulus q. In (8), $v_1 \le v_2 \le v_3$ are the turning points of the motion along the v axis, defined by $V_{HH}(u{=}0, v_i) = e$ $(i = 1, 2, 3)$. The tori bifurcating at the energies e_{lk} have the same v motion as the A orbit: $v_T(t) = v_A(t)$. Their u motion is given by

$$u_T(t) = \sqrt{(e - e_{lk})/3}\,\sin(t + \phi)\,, \qquad e \ge e_{lk}\,, \qquad \phi \in [0, 2\pi)\,. \tag{9}$$

The angle ϕ describes the members of the degenerate families of tori.

According to semiclassical perturbation theory [17], the actions S_{lk} of the tori are changed in first order of ϵ by

$$\delta_1 S_{lk}(\phi) = -\epsilon \oint_{lk} H_1(u_T(t), v_T(t))\,\mathrm{d}t = -\frac{\epsilon}{\alpha^2}\int_0^{T_{lk}^{(0)}} u_T^2(t)\, v_T(t)\,\mathrm{d}t\,, \tag{10}$$

where $T_{lk}^{(0)} = 2\pi k$ are the periods of the unperturbed tori [7]. The integral in (10) takes the form $\delta_1 S_{lk}(\phi) = A_{lk} + B_{lk}\cos(2\phi)$. In the asymptotic limit $e \to 1$, where $q \to 1$ and $T_A \sim \ln[432/(1-e)]$, the coefficients A_{lk} and B_{lk} can be given analytically [15]. Integrating the phase shift caused by $\delta_1 S_{lk}(\phi)$ over the angle ϕ (i.e., over the torus T_{lk}) yields a modulation factor [17] $\mathcal{M}_{lk}$

$$\mathcal{M}_{lk} = \frac{1}{2\pi}\int_0^{2\pi} e^{\frac{i}{\hbar}\delta_1 S_{lk}(\phi)}\,\mathrm{d}\phi = e^{\frac{i}{\hbar}A_{lk}}\, J_0(|B_{lk}|/\hbar)\,, \tag{11}$$

to be inserted under the sum of tori in the trace formula for the unperturbed SHH system given in [7]. Replacing the Bessel function in (11) by its asymptotic form $J_0(x) \sim \sqrt{2/\pi x}\cos(x - \pi/4)$ yields two terms for each torus T_{lk}, corresponding to the two isolated orbits R and L into which it is broken up by the perturbation. Reading off their overall amplitudes $\mathcal{A}_{\mathrm{R,L}}$ in the perturbed trace formula and identifying them with their expression for isolated orbits given in (5), i.e. equating

$$\mathcal{A}_{\mathrm{R,L}} = \frac{1}{\pi\hbar}\,\frac{T_{\mathrm{R,L}}}{l\sqrt{|\mathrm{TrM}_{\mathrm{R,L}} - 2|}} \tag{12}$$

uaing the unperturbed periods $T_{lk}^{(0)}$ for $T_{\mathrm{R,L}}$, we can determine the perturbative expression for the stability traces. For the first repetitions $(l = 1)$ they become

$$\mathrm{TrM}_{\mathrm{R}_n,\mathrm{L}_m}(e) \;\sim\; 2 \mp 5.069\left(\frac{e - e_{1k}}{1 - e_{1k}}\right) \qquad \text{for} \qquad e \to 1\,, \tag{13}$$

and thus have exactly the same functional form as in (6). Here e_{1k} are the bifurcation energies of the primitive A orbit; $k = 2, 3, \dots$ labels the pairs of R_m and L_n orbits with $m = 2k + 1$ and $n = 2k + 2$, and the signs are to be chosen as in (6). In (13) we have put $\epsilon = 1$ which is justified since even for this value the perturbations $\delta_1 S_{lk}$ near $e \sim 1$ are sufficiently small.

Although the perturbative result (13) contains a too small value of the constant 5.069 (instead of 6.183) by 18%, it explains qualitatively correctly the numerical features of the 'HH fans' in (6), in particular the linear intersection of the curves $\mathrm{TrM}_{\mathrm{R,L}}(e)$ at $e = 1$ at two values lying symmetrically to $\mathrm{TrM} = +2$.

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