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On the Padé approximations to the Birkhoff–Gustavson normal form

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Abstract. We demonstrate the efficiency of the Padé approximations to the Birkhoff–Gustavson normal form and to the associated formal integrals of motion for the case of the Hénon–Heiles system. The accuracy of the formal integrals of motion in the regular regions where invariant tori exist is vastly improved, with the tendency that the poles of Padé approximations are located in the chaotic regions of the surface of section. The special case of the integrable Hénon–Heiles system is an excellent example showing that here the poles of the Padé approximations are located in classically forbidden regions. The 14th-order formal integral does not yet agree with the exact (numerical) surface of section, whilst its [5, 5] Padé approximation does (within the limits of graphical resolution). These findings re-confirm the Shirts–Reinhardt picture, and supplement the recent paper by Kaluža and Robnik.

In a recent paper (Kaluža and Robnik 1992; henceforth referred to as KR) we have expounded the method of the Birkhoff–Gustavson normal form, which is suitable and systematic for Hamiltonian systems of N degrees of freedom for which the Hamiltonian can be represented by an N-dimensional harmonic oscillator plus a series of higher-order monomial terms, which make the system's dynamics nonlinear and typically non-integrable and hence chaotic. The method is due originally to Birkhoff (1927) and Gustavson (1966); the method has been further developed by Robnik (1984), see also Eckhardt (1986). We have analysed its applicability in the generic systems of mixed type classical dynamics (typical KAM systems in which the regular regions covered with smooth invariant tori coexist in the energy surface (and surface of section (SOS)) with the chaotic regions), and investigated its convergence and divergence properties in relation to the geometry of the dynamics (phase portrait). In the specific case of the Hénon–Heiles system investigated numerically we have found that the formal integrals of motion (calculated up to and including the 14th order) did behave convergently in the classically regular regions, and even in chaotic regions with short-time clustering characterized by a small value of the finite-time analogue of the Lyapunov exponent. This is surprising since the Birkhoff–Gustavson normal form and the associated formal integrals of motion are of course known, in general, to be at best only an asymptotic series. The significance of our findings in (KR) is thus in showing that under certain conditions the optimal cut-off term in the series can be of very high order, and that the optimally cut-off series can be a good approximation to those invariant tori that still rigorously exist (as KAM tori)†.

† For general comments on the Borel summability and on the approximations to the Borel sums of asymptotic or divergent series see, e.g. Killingbeck (1977) and references therein.

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These results provide additional support for the Shirts–Reinhardt picture (1982; henceforth referred to as SR), employing somewhat simpler tools and analysis. In fact, (SR) have also analysed the scheme of Padé approximations as a suitable re-summation technique for the Birkhoff–Gustavson normal form and for the associated formal integrals. They have shown that this works well, and the goal of the present short paper is to offer additional results demonstrating the usefulness of the Padé approximations†, thereby making the results and conclusions of (SR) more quantitative (cf KR).

We omit all the technical details, the mathematical derivation and the description of the Birkhoff–Gustavson normal form (which can be found in (KR)), and concentrate only on the final results for the classic Hénon–Heiles system (Hénon and Heiles 1964) with two degrees of freedom, defined by

$$H = \tfrac{1}{2}(x_1^2 + x_2^2 + y_1^2 + y_2^2) + \lambda(x_1^2 x_2 + \eta x_2^3) \tag{1}$$

where x_1, x_2 are the coordinates and y_1, y_2 are their conjugate momenta and $\lambda = 1$, $\eta = -\frac{1}{3}$. We shall call the Hamiltonian (1) the generalized Hénon–Heiles Hamiltonian. The unperturbed frequencies are $\omega_1 = \omega_2 = 1$, so there is a 1-fold resonance.

The commensurability matrix has the matrix elements $a_{11} = 1$, $a_{12} = -1$. According to Gustavson (see equation (7) in (KR)) the formal integral of motion is

$$I = I_1 = \tau_1 + \tau_2 = \tfrac{1}{2}(\tilde{x}_1^2 + \tilde{y}_1^2 + \tilde{x}_2^2 + \tilde{y}_2^2) \tag{2}$$

where $\tilde{x}_i$ and $\tilde{y}_i$ are the transformed final coordinates and momenta, respectively. As is customarily done in the literature (Gustavson 1966, SR, KR) we define the integral of motion as

$$K = I - H. \tag{3}$$

We have used the symbolic algebra program (Kaluža 1993), written in the programming language REDUCE (Hearn 1987), to calculate the series of the normal form Hamiltonian and of the approximate integrals of motion for the generalized Hénon–Heiles system. The program works for any Hamiltonian system with polynomial potential with a non-vanishing harmonic part, and for any number of degrees of freedom. The calculation for the two-dimensional Hénon–Heiles system provides a good test of the code. We have checked all numerical coefficients given in Gustavson (1966) and found a perfect agreement, except for the following well understood differences: there is a single sign error in the coefficient $I(185)$ for the integral of motion in his table IV, and a number of differences in coefficients of the normal form Hamiltonian and the approximate integral in higher orders, which most probably come from the roundoff errors and their propagation in his numerical procedure. Kaluža's program (Kaluža 1993) is written in REDUCE with infinite precision and is as general as possible, so that his scheme is certainly better than Gustavson's (1966) and Giorgilli's (1979) (both written in FORTRAN), since sometimes in the latter ones the accumulated numerical roundoff errors can be considerable. As one

† For one-dimensional systems a similar analysis has been extensively performed by Ali *et al* (1986). However, one-dimensional systems are always integrable (and also ergodic!), and never show a chaotic behaviour, so the applicability of the Birkhoff–Gustavson normal form is at the same time rather straightforward and very successful.

example, Gustavson's (1966) coefficient $I(427) = 70.817\,255$ should read 70.817 274. We are absolutely confident that Kaluža's program is flawless.

The fourth-order integral $K^{(4)}$ has the following expression in terms of original variables on the surface of section (SOS), defined by $x_1 = 0$ and $y_1 > 0$

$$K^{(4)}|_{\mathrm{SOS}} = \frac{\lambda^2}{48}(45\eta^2(x_2^2 + y_2^2)^2 + 6\eta(7x_2^2 + 5y_2^2)y_1^2 + (-4x_2^2 + 20y_2^2 + 5y_1^2)y_1^2). \tag{4}$$

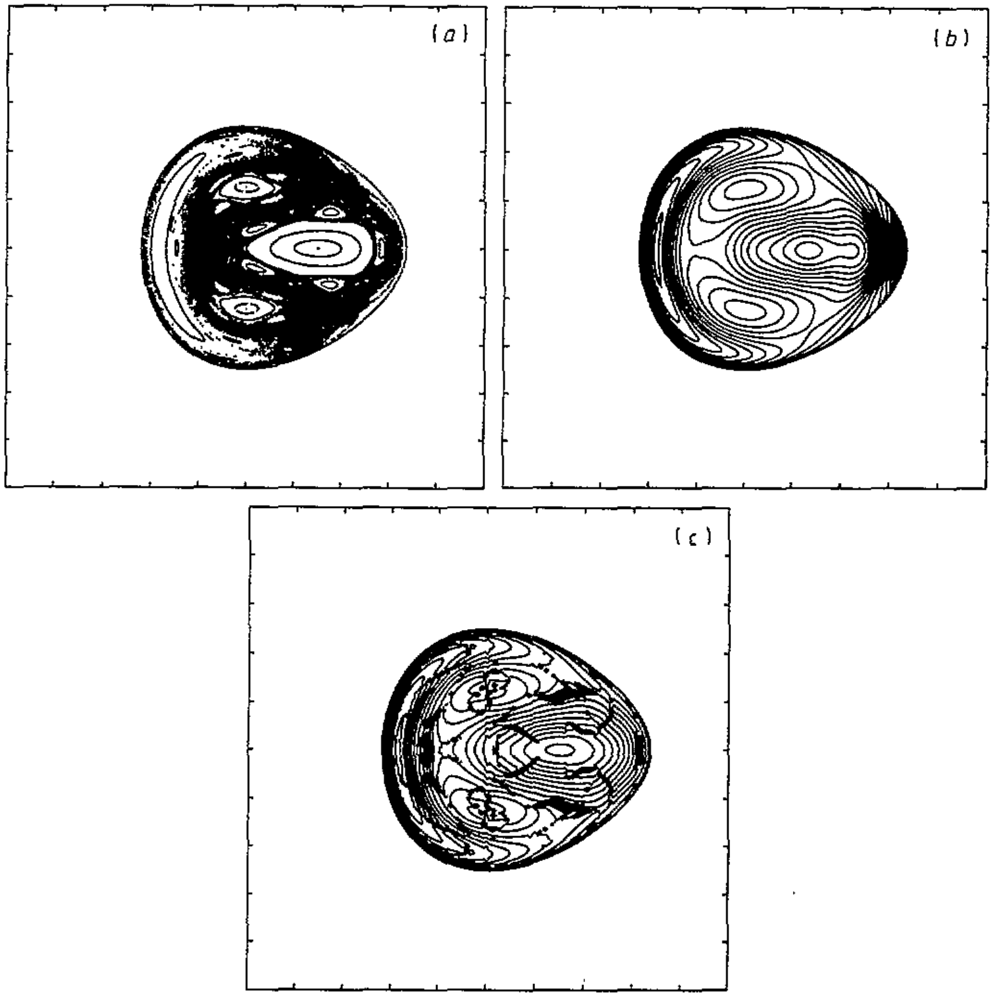


Figure 1. The SOS for the Hénon–Heiles system at the energy $E = 1/8$ ($\approx$ critical energy). (a) The exact (numerical) Poincaré plot. (b) The curves of constant value of the approximate integral of motion $K^{(14)} = I^{(14)} - H$ (14th order). (c) The same-height contours of the [5, 5] Padé approximant (to the 14th-order formal integral).

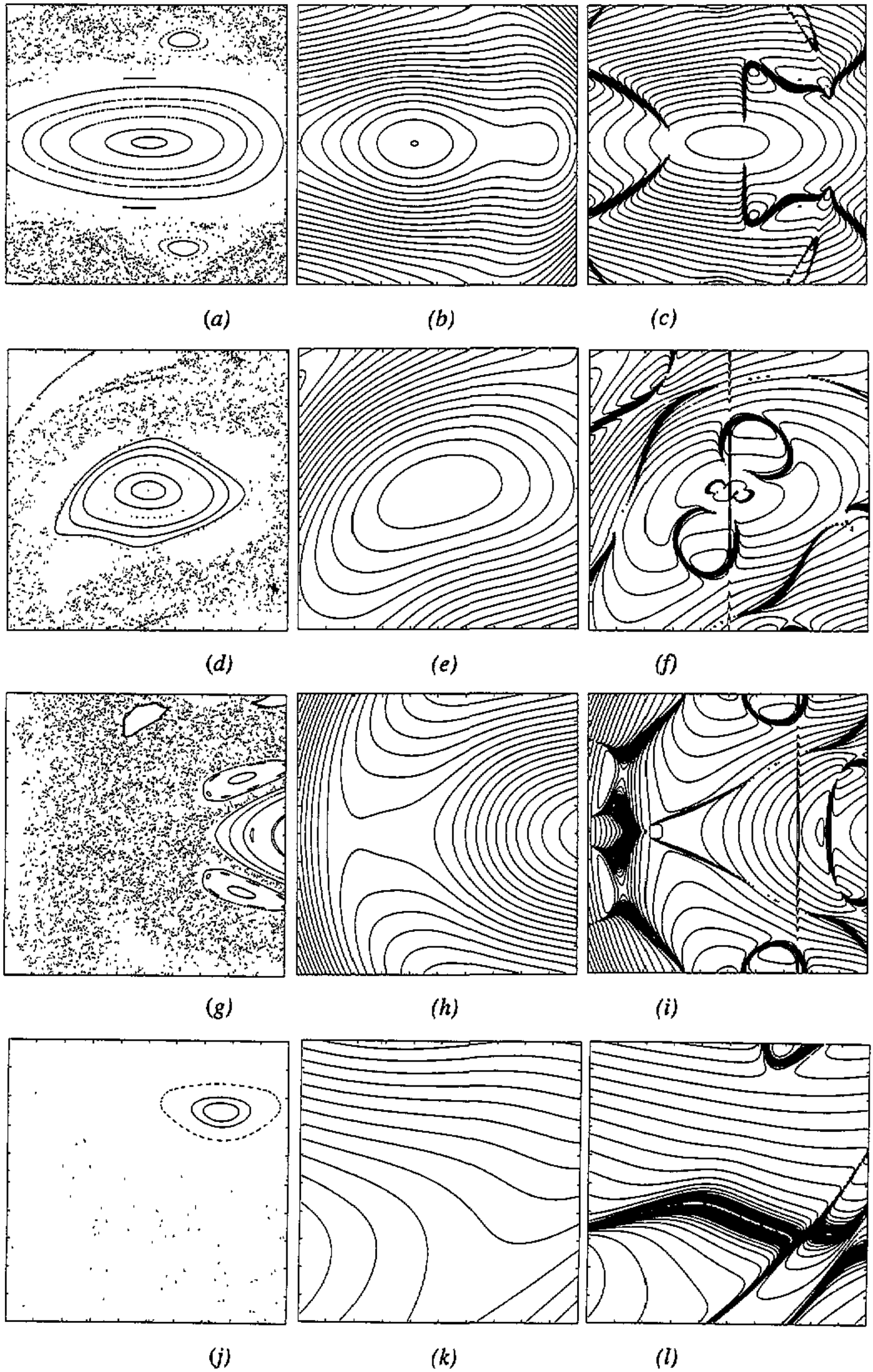
The curves in (a) are obtained using a fourth-order Runge–Kutta integration method with the time step $h = 0.001$. The parameters of the Hénon–Heiles Hamiltonian are $\lambda = 1$, $\eta = -1/3$. The surface of section is defined by the conditions $x_1 = 0$ and $y_1 > 0$. The x axis represents the coordinate x_2 and the y axis represents the momentum y_2. The range of both quantities is $[-1.0, 1.0]$. Note the tendency of the poles of the Padé approximations to cluster in the chaotic regions. Also, the central region of the largest stability island shown in (a) is described much better by the [5, 5] Padé approximant than by the 14th-order formal integral itself.

We have been able to obtain the approximate integrals up to and including the fourteenth order in powers of coordinates and momenta. This is one order beyond the previously published results for the Hénon–Heiles system (SR). The result enables me to calculate (in the present short paper) the Padé approximations (of order [5, 5]), to the 14th-order formal integral $K^{(14)}$ using the very efficient so called *epsilon algorithm* (Wynn 1956, Macdonald 1964). This is again one order higher than in (SR) (see also Shirts and Reinhardt 1981) and in Jaffe and Reinhardt (1982). I do not consider the non-diagonal approximants $[L, M]$, where L differs from M, since there is no deep reason to do so. On the contrary, it is expected that the degree and quality of approximation is best in the case of the diagonal approximants.

In figure 1(*a*) we show the Poincaré plot on the SOS of the classic Hénon–Heiles system at energy $E = 1/8 = 0.125$ ($\approx$ critical energy). The contours of the 14th-order formal integral are shown in figure 1(*b*), and the same height contours of the corresponding [5, 5] Padé approximation are given in figure 1(*c*). Of course, the poles are marked simply by the high density contours. As is readily seen the poles of the Padé approximant show a tendency to be located within the chaotic regions. This is intuitively obvious since in the regular regions there might exist smooth *local* integrals of motion, but it is good to have the confirmation. As the order of the formal integral of motion increases, so that the order M of the Padé approximations $[M, M]$ can be increased, one expects that the poles will move to chaotic regions, and the Padé approximations are expected to become better and better in the regular regions, even if the formal integrals themselves actually diverge. The Padé approximations are thus an efficient approximation to the *local* KAM integrals of motion. One *should observe that the central region of the largest stability island in figure 1 is significantly* better described by the Padé approximant [5, 5] than by the 14th-order formal integral from which it is derived. Thus, the Padé approximations are significant and efficient.

In figure 2(*a*)–(*c*) we show the magnified central region of the largest stability island of figure 1(*a*), together with contours of constant 14th-order formal integral in figure 1(*b*) and the same height contours of the [5, 5] Padé approximant. We also show three other magnified small regions of figure 1(*a*), in figure 2(*d*)–(*f*), (*g*)–(*i*) and (*j*)–(*l*). The general conclusion is that the Padé approximations do indeed improve the quality of the approximation to the formal integrals as obtained by the Birkhoff–Gustavson normal form, and that there is a general tendency to push the poles into the chaotic regions, so that in the regular regions the Padé approximations are smooth at sufficiently high order. At the same time we see how difficult it is to capture the fine structure of the small regular regions. Obviously, much higher orders of Padé approximations are needed to achieve this.

Figure 2. (Opposite) The applicability of the formal integral of motion (14th order) and of the [5, 5] Padé approximations of the Hénon–Heiles system at the energy $E = 1/8 \approx$ critical energy, in four small and magnified regions of figure 1. In parts (*a*), (*d*), (*g*), (*j*) (the first column, *from top to bottom) we show the Poincaré plots, in* (*b*), (*e*), (*h*), (*k*) (*the second column*) the contours of constant value of the 14th-order formal integral, and in parts (*c*), (*f*), (*i*), (*l*) (the third column) the contours of the same constant value of the [5, 5] Padé approximations. The contours with values from -0.020 to 0.020 in steps of 0.0005 are shown. The parameters of the Hénon–Heiles Hamiltonian are $\lambda = 1$, $\eta = -1/3$. The surface of section is defined by the conditions $x_1 = 0$ and $y_1 > 0$. The x axis represents the coordinate x_2 and the y axis represents the momentum y_2. The range of both quantities is: $[0.1, 0.5] \times [-0.2, 0.2]$ in (*a*)–(*c*) (the first row); $[-0.2, 0.2] \times [0.1, 0.4]$ in (*d*)–(*f*) (the second row); $[-0.3, 0.1] \times [-0.2, 0.2]$ in (*g*)–(*i*) (the third row); $[0.2, 0.4] \times [-0.3, -0.1]$ in (*j*)–(*l*) (the fourth row). In (*a*)–(*c*) it is seen that the Padé approximation yields a considerably improved description of this central region of the largest stability island (seen in figure 1(*a*)). The general trend of the poles of Padé approximations to cluster in the chaotic regions is clearly visible.



Finally, we present the results for the special case of the integrable Hénon–Heiles system, which is the special case of the generalized Hénon–Heiles system (1) for any λ and $\eta = 2$. This system is well known to be integrable (Bountis *et al* 1982). The exact integral of motion can be expressed as

$$I_e = \lambda^2 x_1^4 + 4\lambda^2 x_1^2 x_2^2 - 4\lambda y_1 (y_1 x_2 - y_2 x_1) + 4\lambda x_1^2 x_2 + 3(y_1^2 + x_1^2). \qquad (5)$$

In figure 3(*a*) we show the exact Poincaré plot in the SOS for this system with $\lambda = -1$, at the energy $E = 0.004$, identical to the corresponding contours of the exact integral of motion (5). In figure 3(*b*) the corresponding contours of the 14th-order formal integral of motion are shown, and in figure 3(*c*) the same height contours of the [5, 5] Padé approximant are

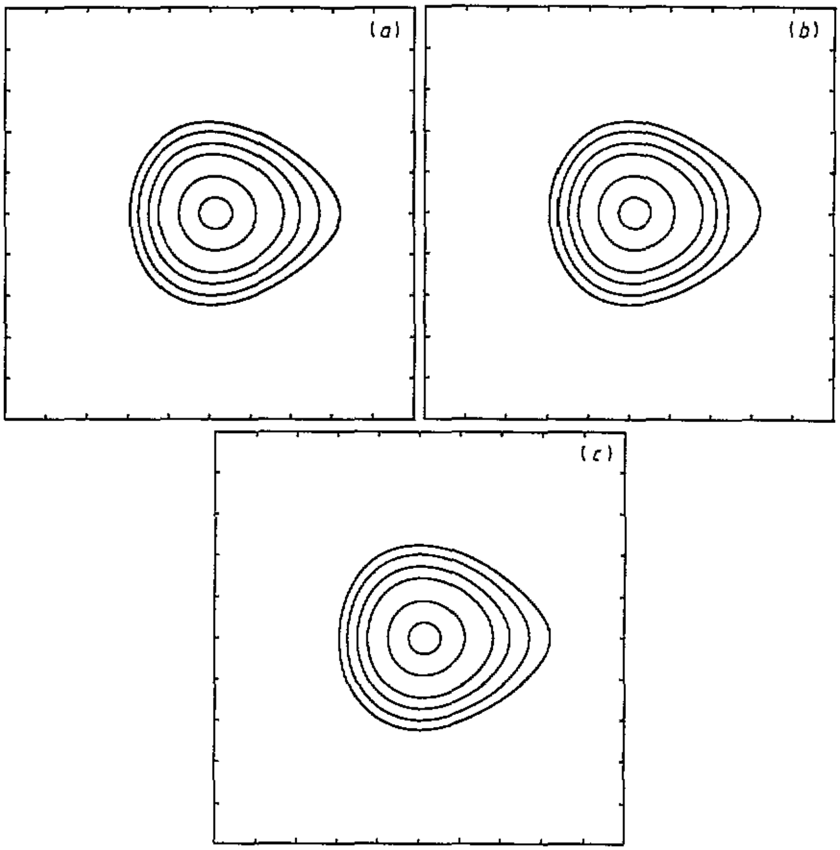


Figure 3. The applicability of the 14th-order formal integral of motion and the corresponding [5, 5] Padé approximant for the integrable Hénon–Heiles system (1) with $\lambda = -1$, and $\eta = 2$ at energy $E = 0.004$. (*a*) The Poincaré plot on the SOS as obtained by exact numerical integration, and also by the contours of the exact integral of motion (5). (*b*) The curves of constant value of the 14th-order formal integral of motion $K^{(14)} = I^{(14)} - H$ as obtained by the Birkhoff–Gustavson normal form procedure. (*c*) The same height contours of the [5, 5] Padé approximant to the 14th-order formal integral of motion. The contours with values from −0.020 to 0.020 in steps of 0.001 are shown. The surface of section is defined by the conditions $x_1 = 0$ and $y_1 > 0$. The x axis represents the coordinate x_2 and the y axis represents the momentum y_2. The range of both quantities is [−0.2, 0.2]. It should be emphasized that there are no poles of the Padé approximant inside the allowed region in the SOS, i.e. they are located strictly in classically forbidden regions in the phase space.

given. It should be noted that there are no poles inside the classically allowed region in the SOS (so they are located in the classically forbidden regions), and that the Padé approximant does not differ from the exact contours whereas the 14th-order formal integral of motion is not yet satisfactory, since it significantly deviates from the exact curves at the rightmost parts of the contours.

These findings do confirm the usefulness of the Padé approximations in improving the convergence and accuracy of the formal integrals of motion obtained within the framework of the Birkhoff–Gustavson normal form procedure. In particular, they confirm the Shirts–Reinhardt (SR) picture, and indicate that further research might give us even better tools to construct an efficient and systematic approximation to the integrals of motion where they do still exist locally (in the sense of the KAM theory). One additional theoretical step towards this goal might also be assisted by the approach of Bogomolny (1983, 1984), where the singularities of the perturbation series are associated with and related to the periodic orbits: the perturbation series has a '... singularity of the type of the square root of some quadratic form near each periodic trajectory of the considered problem'. In this regard it would be helpful to obtain even higher orders of the formal integrals, for which one could explicitly employ the special symmetries of the Hénon–Heiles system (see Finkler *et al* 1991).

It should be noticed that the Birkhoff–Gustavson normal form approach has been successful in classical, semiclassical and quantum applications for the Hénon–Heiles system (SR, Jaffe and Reinhardt 1982, Swimm and Delos 1979, Noid and Marcus 1977, Robnik 1984, KR) and in the hydrogen atom in a strong magnetic field (Robnik 1981, 1982, Hasegawa *et al* 1989, Robnik and Schrüfer 1985, Kuwata *et al* 1990), and also in the one-dimensional anharmonic oscillators (Ali and Wood 1989, Ali and Snider 1989). The significance of such studies may be underlined by the remark that very often the classical perturbation series (normal form) converge in the regions where the quantum perturbation series diverge, and in such cases the study of semiclassical approximations is especially instructive and useful. It might give us new clues towards the re-summation techniques in quantum perturbation methods. In general, further progress in this field might be very fruitful.

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