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On the limitations of the Birkhoff–Gustavson normal form approach

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Abstract. Recently, the Birkhoff-Gustavson normal form (BGNF) approach has been used in both classical and semiclassical calculations. In this paper, we consider the limitations associated with this approach. At the classical level, we emphasise the need to properly take into account the divergence properties of the BGNF series. By reviewing an earlier work we demonstrate that this divergence problem may, in some cases, be resolved. However, after considering several standard quantisation rules, we find that it is not possible to obtain the correct quantisation of a system via the BGNF. As a result, we maintain that care should be used when working with the BGNF.

1. Introduction

The classical Birkhoff-Gustavson normal form (BGNF) (Birkhoff 1927, Gustavson 1966) and its semiclassical quantisation have received considerable attention in recent years (Churchill *et al* 1978, Jaffé and Reinhardt 1982, Robnik 1984, Robnik and Schrüfer 1985, Ali 1985). The following features of the BGNF approach (for classical and semiclassical descriptions of dynamical systems) make it quite appealing: (i) the BGNF series can be obtained by the elegant Lie transformation method that is very general in nature, (ii) the BGNF series is the classical analogue of the quantum Rayleigh-Schrödinger (RS) perturbation series and (iii) the BGNF approach provides approximate classical constants of motion and semiclassical results in some cases where such results may be difficult to obtain otherwise. In spite of these appealing features, the BGNF approach has severe limitations that have not been properly emphasised in earlier work. Our purpose here is to illustrate some of the shortcomings of the BGNF approach.

The two primary reasons for the limited range of application of the BGNF approach are (i) the common divergence of and (ii) the difficulty in the quantisation of the BGNF series. For a given perturbed system, the BGNF series necessarily diverges if the system is non-integrable and may diverge *even if the system is integrable.* Hence, one often finds that the series is divergent. In addition, while semiclassical results may approach the correct eigenvalues of the nth quantum state as n becomes very large, there is no method currently available for obtaining the correct quantum description from the BGNF for all n. This is due to the fact that the question of the quantisation of a classical Hamiltonian system containing the canonical variables q and p in the form $q^{\alpha}p^{\beta}$, with α, $\beta \geq 2$, is still open. We illustrate these limitations with the help of a model system.

2. The BGNF of an anharmonic oscillator

In a previous paper (Ali *et al* 1986, hereafter referred to as I) we studied the BGNF series for the quartic anharmonic oscillator $H=\frac{1}{2}(p^2+x^2+gx^4)$. The BGNF K of H was obtained by canonically transforming the variables (x, p) to (ξ, η). This transformation was achieved by employing the method of Lie transformations, by means of which we generated 50 terms for $K=UK_0$. The lower order terms of this alternating series were found to be

$$U=1+\tfrac{3}{4}y-\tfrac{17}{16}y^2+\tfrac{375}{128}y^3-\tfrac{10\,689}{1024}y^4+\tfrac{87\,549}{2048}y^5-\tfrac{3132\,399}{16\,384}y^6+\tfrac{238\,225\,977}{262\,144}y^7\ldots \tag{1}$$

where

$$y=gK_0 \qquad K_0=\tfrac{1}{2}(\xi^2+\eta^2)$$

the harmonic oscillator action. We find it convenient to perform the canonical transformation

$$Q=2^{-1/2}(\xi-\mathrm{i}\eta) \qquad P=2^{-1/2}(-\mathrm{i}\xi+\eta) \tag{2}$$

so that the transformed Hamiltonian K becomes a power series in $y=\mathrm{i}gQP$. We recently discovered that the first three terms in our BGNF series were given in an earlier paper (Carhart 1971). From the few terms with which he worked, Carhart was not able to deduce the convergence properties of the BGNF series—a situation that is more common than not.

The rapid growth of the coefficients in equation (1) indicates that the series for K may not converge for all y. In fact, in a study of this classical BGNF (I), we found that the series has a small radius of convergence ($y_0=0.116\,16\ldots$). Thus, for this *integrable system*, the BGNF series has the limited range of application $0\leqslant y<0.116\,16\ldots$. The fact that the BGNF series diverges for $y\geqslant y_0$ does not refute the global integrability of H. The situation is much worse when the system does not support the required number of constants of motion, i.e. when the system is non-integrable, as the series for K does not converge to H in this case. The reason for this is that K is integrable by construction while H is non-integrable by assumption, and hence $H\neq K$. For integrable situations, where the radius of convergence is non-zero (Robnik 1984), the usefulness of the BGNF may be increased by appropriately summing the series. For our model anharmonic oscillator, we have summed the divergent BGNF series (equation (1)) by the method of Padé approximants (Baker 1975), chosen in such a manner as to yield the known asymptotic limits. The procedure to determine these Padé approximants is (see I)

(i) define the cube of the series U to be Z, i.e. $Z=U^3$;
(ii) determine the $[m+1, m]$ Padé approximant of Z, $P[m+1, m]$, and
(iii) then $K\approx K_0\{P[m+1, m]\}^{1/3}$.

Since the rate of convergence of these approximants is rather slow as m increases, we developed an 'asymptotic' series for our function by first identifying the BGNF with a generalised hypergeometric function (Codaccioni and Caboz 1984), for which the analytical continuation is well known, and then finding an appropriate Padé approximant of the analytically continued hypergeometric function. The leading terms in this analytically continued series are

$$V=1-\tfrac{4}{3}cz+(\tfrac{2}{3}c^2-\tfrac{1}{16})z^2-\tfrac{8}{81}c^3z^3-(\tfrac{5}{243}c^4-\tfrac{1}{3072})z^4+\tfrac{1}{1920}cz^5+(\tfrac{14}{6561}c^6+\tfrac{7}{13\,824}c^2)z^6\ldots \tag{3}$$

where

$$K=\frac{1}{gz^2}V \qquad z=(\alpha y)^{-2/3} \qquad \alpha=\frac{3\Gamma(\frac{3}{4})^2}{\pi^{1/2}2^{5/4}} \qquad c=-\frac{3\Gamma(\frac{3}{4})^4}{\pi^2 2^{3/2}}.$$

The procedure to determine the asymptotic Padé approximants is (again see I)

(i) determine the $[j,j]$ Padé approximants, $P_a[j,j]$, of equation (3), and

(ii) then $K=(1/gz^2)P_a[j,j]$.

By representing our function by the two Padé approximants $P[14,13]$ and $P_a[14,14]$, we were able to obtain excellent values for the period of the anharmonic oscillator. With the divergence problem for our example thus resolved, we now turn our attention to the problem of obtaining quantum results from the BGNF. For a discussion of the divergence problem in a multidimensional case, see Bogomol'nyĭ (1983).

3. The quantisation of the BGNF

In the previous section we have seen that the range of correct classical results in the BGNF approach is limited by the radius of convergence of the BGNF series and that this limitation may be removed by summing the series, providing it is summable. However, the solution of this classical problem does not resolve the additional and independent problem of obtaining the correct quantum description of a system from the BGNF. Robnik (1984) has pointed out that, because the BGNF series (whether convergent or divergent) contains terms of the form $q^\alpha p^\beta$ with α, $\beta \geqslant 2$, there is no unique solution to the quantisation problem. In this section we illustrate the limitations of several practical alternatives to exactly quantising the BGNF.

The quantisation rule $p\to \boldsymbol{p}=-\mathrm{i}\hbar\,\mathrm{d}/\mathrm{d}x$ and $x\to \boldsymbol{x}$, yields the unique operator

$$\boldsymbol{H}=\tfrac{1}{2}[-\hbar^2(\mathrm{d}^2/\mathrm{d}x^2)+\boldsymbol{x}^2+g\boldsymbol{x}^4] \qquad (4)$$

for the classical anharmonic oscillator Hamiltonian $H(x,p)$, where $-\infty\leqslant x\leqslant\infty$ and $-\infty\leqslant p\leqslant\infty$. We accept, as is generally done, $\boldsymbol{H}(\boldsymbol{x},\boldsymbol{p})$ as the correct quantum operator associated with $H(x,p)$, i.e. we assume that $\boldsymbol{H}$ provides the correct energy spectrum. The eigenvalues of $\boldsymbol{H}$ can be accurately calculated by such methods as matrix diagonalisation, WKBJ calculations and the summation of the RS perturbation series. The problem with the quantisation of the BGNF is the following. At present, there does not exist any method by which the correct energy spectrum of $\boldsymbol{H}$ may be obtained from the BGNF series *or* its summation. This drawback of the BGNF approach is a direct consequence of the fact that K contains terms of the form $Q^\alpha P^\beta$ with α, $\beta\geqslant 2$. The question of how to obtain the correct quantum operator corresponding to a classical Hamiltonian containing such terms is still open. In the remainder of this section we shall illustrate that this is the case by demonstrating, for our model system, the limitations of several approaches to the problem. We restrict our discussion to these commonly used approaches as others, such as geometric quantisation (Simms 1977), are not yet in final form.

3.1. *Semiclassical (torus) quantisation*

One method that may be used to obtain quantum results is to determine a semiclassical expansion in $\hbar$ around the BGNF Hamiltonian. Since K, the BGNF Hamiltonian for our (one-dimensional) model system, is a function of the action K_0, the first-order semiclassical or torus quantisation (Percival 1977, Jaffé and Reinhardt 1982) of the system is simple; it is obtained by replacing K_0 by $(n+\frac{1}{2})\hbar$, as we have set $\omega = 1$. (For multidimensional systems, the BGNF is a function of the action variables only if the system is non-resonant. Nevertheless, torus quantisation is straightforward even in the multidimensional case.) Since either the series *or* the Padé approximants can be quantised by the torus quantisation method, the classical solution of the divergence problem can be used here. However, while the torus quantisation of our Padé approximants does approach the correct eigenvalues as $n \to \infty$ for finite g, it yields poor results for the combination of small n and appreciable g (see table IV in I). In particular, the often studied ground-state results are poorly reproduced by this first-order semiclassical quantisation. In order to improve on this approach one could determine higher-order terms in the semiclassical expansion. However, the simplicity in the torus quantisation of the Padé approximants is lost in this case and the divergence of the classical BGNF again becomes a problem.

3.2. Quantisation via correspondence rules

In quantum mechanics, the usual method used to obtain the operator corresponding to a classical Hamiltonian that contains products of the form $q^\alpha p^\beta$ is to supplement the general quantisation rule $p \to \boldsymbol{p} = -\mathrm{i}\hbar\nabla$ and $q \to \boldsymbol{q}$ with a linear correspondence rule. This additional rule, which symmetrises the operator so as to make it Hermitian, is required in order to maintain the basic postulates of quantum mechanics. When α, $\beta = 1$, the standard correspondence rules, e.g. symmetrisation, Weyl–McCoy and Born–Jordan (Mayes and Dowker 1972), yield the Hermitian operator $\frac{1}{2}(\boldsymbol{qp}+\boldsymbol{pq})$, which does have empirical support. However, when α, $\beta \geqslant 2$, these rules yield different operators 'corresponding' to a given classical Hamiltonian. In principle, there is a very large number of rules from which to choose (Cohen 1966), all of which yield Hermitian operators; in practice, a particular rule may be chosen on the basis of further critieria (Springborg 1983). However, while a given rule may be judged 'better' than another, it has been shown (Abraham and Marsden 1978) that none can yield the (unique) correct Hamiltonian operator when α, $\beta \geqslant 2$. We verify this result by quantising our model system using the above standard rules, of which a modified Weyl–McCoy rule has previously been applied to a BGNF (Robnik 1984, Robnik and Schrüfer 1985).

Unfortunately the correspondence rules, defined below, cannot be applied directly to the Padé approximants (or the asymptotic series) given in § 2 as these functions are not polynomials in Q and P. (Recall that torus quantisation can be applied directly to the Padé approximants.) Hence, the resolution of the classical divergence problem is of no benefit in this quantisation procedure. As a result, one must quantise the BGNF series and then, if possible, sum the resulting quantised series. Since the quantum RS series and its summation for the quartic anharmonic oscillator have been studied extensively (see, e.g., Bender and Wu 1969, 1976, Simon 1970, Graffi *et al* 1970), we do not sum the quantum series obtained via the different correspondence rules but rather compare these series with the RS series. That this comparison indicates whether a given correspondence rule yields the correct quantisation follows from the fact that there is a unique power series, in a given coupling constant, whose summation yields the correct eigenvalues. The ground-state RS series given by Bender and Wu (1969) has been summed to the correct eigenvalues by the Borel summation method (Graffi *et al* 1970).

We begin by giving the different correspondence rules.

(i) Weyl-McCoy rule:

$$q^{\alpha}p^{\beta} \rightarrow \frac{1}{2^{\beta}} \sum_{\gamma=0}^{\beta} \binom{\beta}{\gamma} \boldsymbol{p}^{\gamma}\boldsymbol{q}^{\alpha}\boldsymbol{p}^{\beta-\gamma} \tag{5}$$

or in standard order ($\boldsymbol{q}$ to the left of $\boldsymbol{p}$),

$$q^{\alpha}p^{\beta} \rightarrow \sum_{\gamma=0}^{\min(\alpha,\beta)} \frac{(-\mathrm{i}\hbar)^{\gamma}\gamma!}{2^{\gamma}} \binom{\alpha}{\gamma}\binom{\beta}{\gamma} \boldsymbol{q}^{\alpha-\gamma}\boldsymbol{p}^{\beta-\gamma}. \tag{6}$$

(ii) Born-Jordan rule:

$$q^{\alpha}p^{\beta} \rightarrow \frac{1}{\beta+1} \sum_{\gamma=0}^{\beta} \boldsymbol{p}^{\gamma}\boldsymbol{q}^{\alpha}\boldsymbol{p}^{\beta-\gamma}. \tag{7}$$

(iii) symmetrisation rule:

$$q^{\alpha}p^{\beta} \rightarrow \tfrac{1}{2}(\boldsymbol{q}^{\alpha}\boldsymbol{p}^{\beta} + \boldsymbol{p}^{\beta}\boldsymbol{q}^{\alpha}). \tag{8}$$

The quantisation of a BGNF series for a given correspondence rule is achieved by applying that rule to the series, *term by term.* The quantum perturbation series (a series in the coupling constant g, with each term being some function of the quantum number n) is then obtained by acting on a state vector with the resulting series of operators. By identifying P and Q with the annihilation and creation operators of the harmonic oscillator basis, the application of this procedure to our BGNF (equation (1)) is straightforward. Below, we give the first few terms of the ground-state ($n=0$) series for each of the above rules, as well as for the torus quantisation. The RS series was obtained from Bender and Wu's coefficients by setting their $\lambda = \frac{1}{2}g$. The coefficients in the series are given with common denominators for ease of comparison:

RS: $E_0 = \frac{1}{2}\hbar + \frac{6}{16}g\hbar^2 - \frac{84}{128}g^2\hbar^3 + \frac{5328}{2048}g^3\hbar^4 - \frac{494\,160}{32\,768}g^4\hbar^5 + \frac{14\,667\,696}{131\,072}g^5\hbar^6$

torus: $E_0 = \frac{1}{2}\hbar + \frac{3}{16}g\hbar^2 - \frac{17}{128}g^2\hbar^3 + \frac{375}{2048}g^3\hbar^4 - \frac{10\,689}{32\,768}g^4\hbar^5 + \frac{87\,549}{131\,072}g^5\hbar^6$

Weyl: $E_0 = \frac{1}{2}\hbar + \frac{6}{16}g\hbar^2 - \frac{102}{128}g^2\hbar^3 + \frac{9000}{2048}g^3\hbar^4 - \frac{1282\,680}{32\,768}g^4\hbar^5 + \frac{63\,035\,280}{131\,072}g^5\hbar^6$

Born: $E_0 = \frac{1}{2}\hbar + \frac{8}{16}g\hbar^2 - \frac{204}{128}g^2\hbar^3 + \frac{28\,800}{2048}g^3\hbar^4 - \frac{6840\,960}{32\,768}g^4\hbar^5 + \frac{576\,322\,560}{131\,072}g^5\hbar^6$

symmetric: $E_0 = \frac{1}{2}\hbar + \frac{12}{16}g\hbar^2 - \frac{408}{128}g^2\hbar^3 + \frac{72\,000}{2048}g^3\hbar^4 - \frac{20\,522\,880}{32\,768}g^4\hbar^5 + \frac{2017\,128\,960}{131\,072}g^5\hbar^6.$

(Both forms of Weyl ordering, equations (5) and (6), give the same quantum series above.) By comparing the different series obtained from the BGNF with the RS series, we observe that the Weyl-McCoy series has the same coefficients to first order in the coupling constant, whereas the coefficients of the remaining series are the same only when there is no perturbation, i.e. $g=0$. Thus, if one were to retain just the first two terms of the above series, the Weyl-McCoy series would be the only series that would coincide with the RS series. In this sense, the Weyl-McCoy rule has given the best quantisation, a result that supports the choice of this rule in previous works. However, we stress that, even if it proves possible to sum this series, the summation *cannot* yield the correct eigenvalues. Besides this problem, one is also faced with the difficulty of handling the large number of terms that result from applying a given correspondence rule term by term. It has been suggested (Robnik 1984) that this problem might be dealt with by making the further approximation of modifying the Weyl-McCoy rule by imposing the 'squaring axiom': if $f(q,p) \rightarrow f(\boldsymbol{q},\boldsymbol{p})$, then $f^2(q,p) \rightarrow f^2(\boldsymbol{q},\boldsymbol{p})$. This further approximation, which reduces the Weyl-McCoy rule to torus quantisation in the one-dimensional or multidimensional non-resonant cases, imposes a significant reduction in the accuracy of the ground-state eigenvalues in our example; the first-order coefficient in the torus series above is incorrect. In the case where the correct quantum results for a system are not known, the effect that the squaring axiom has on the accuracy of the approximate results cannot be determined.

The physical reason that no correspondence rule yields the correct quantisation of a BGNF is a result of the form of the Hamiltonian K. Usually, one quantises the *complete* Hamiltonian expressed as $H(q, p) = p^2/2m + V$, where V may contain a term of the form qp, although it is generally just a function of q. However, in the BGNF approach the Hamiltonian is usually an infinite power series in the canonical variables qp and only a truncated part of this series is quantised term by term. That the quantisation of only part of the complete Hamiltonian via a correspondence rule must yield incorrect results is evident from the following considerations.

Paper II (Ali 1985) reports a study of the general anharmonic oscillator $H = \frac{1}{2}(p^2 + x^2 + 2bx^3 + gx^4)$, where we have set $\omega = 1$ here. The first three terms in the BGNF series were found to be

$$K = K_0 + (\tfrac{3}{4}g - \tfrac{15}{4}b^2)K_0^2 + (\tfrac{225}{8}gb^2 - \tfrac{17}{16}g^2 - \tfrac{705}{16}b^4)K_0^3 \tag{9}$$

where K_0 is the harmonic oscillator action. The quantum RS perturbation series (to third order) for this general anharmonic oscillator is

$$\begin{aligned} E = (n+\tfrac{1}{2})\hbar + [\tfrac{3}{4}g(n^2+n+\tfrac{1}{2}) - \tfrac{15}{4}b^2(n^2+n+\tfrac{11}{30})]\hbar^2 + [-\tfrac{1}{96}g^2(102n^3+153n^2+177n+63) \\ + \tfrac{1}{48}gb^2(1350n^3+2025n^2+1701n+513) \\ - \tfrac{1}{96}b^4(4230n^3+6345n^2+4905n+1395)]\hbar^3. \end{aligned} \tag{10}$$

It is clear that the term by term quantisation of the canonical variables in K_0^α for $\alpha \geq 2$ yields different results for the quartic anharmonic oscillator ($b = 0$) and the cubic anharmonic oscillator ($g = 0$). For example

$$b = 0: \quad K_0^2 \to (n^2 + n + \tfrac{1}{2})\hbar^2$$

$$g = 0: \quad K_0^2 \to (n^2 + n + \tfrac{11}{30})\hbar^2.$$

This result is usually explained by means of the Feynman diagram technique. For a given perturbed system, the mth term in the RS series may be determined by summing all connected Feynman diagrams of the corresponding field theory that have no external legs (see, e.g., Fetter and Walecka 1971). Bender and Wu (1969) have demonstrated this for the quartic anharmonic oscillator (ϕ^4 theory). Thus, one expects the different quantisations of K_0^2 above since the Feynman diagrams are different for the ϕ^3 and ϕ^4 theories. The Feynman diagram technique allows one to correctly determine the coefficients in a perturbation series because it takes into account the physical symmetries associated with a given system, i.e. with the *complete* Hamiltonian.

The correspondence rules do not take into account the physical properties of the system; rather, they associate a mathematical symmetry number to each power of K_0. As a result, *no* correspondence rule can quantise the BGNF of the general anharmonic oscillator ($b \neq 0$, $g \neq 0$ in equation (9)) term by term so as to yield the RS series, equation (10). In our earlier work (II) we showed that for $n = 0$ and small values of b and g, the RS series (equation (10)) reproduced the correct energies. We also found that, for these values of b and g, the BGNF series (equation (9)) did not diverge. Thus, the failure to obtain the correct quantum results from a convergent BGNF series is due to the quantisation problem.

3.3. Path integral quantisation

The path integral approach to quantisation, which includes a wide range of topics, is a very active field today. As we are interested in the quantisation of a BGNF, we are constrained to consider the path integral in phase space. In particular, we consider how the operator ordering problem discussed in § 3.2 appears in this formalism. It is generally accepted (see, e.g., Faddeev and Slavnov 1980, Schulman 1981) that the ordering problem is inherent in the phase space path integral and that it becomes evident when one defines the integration procedure in a concrete manner. When the path integral is defined in terms of a measure, as Feynman's original definition was (Feynman 1951), a *limiting procedure* must be chosen in order to evaluate the integral, e.g. the midpoint rule may be used, where one evaluates the Hamiltonian at the midpoint of each discrete interval. Cohen (1970) and Testa (1971) have shown that different definitions of the limiting procedure correspond to different ordering rules, e.g. the midpoint rule corresponds to the Weyl-McCoy rule. When the path integral is defined in terms of a prodistribution (DeWitt-Morette *et al* 1979), one obtains integrands that contain products of coordinates and momenta *at the same time*. Here again, these integrals are not defined until a (time) ordering has been specified (Mizrahi 1981). Hence, the phase space path integral in either form does not resolve the ordering problem, and as a result of this, coupled with the technical difficulties involved with this formalism, we do not consider it further.

4. Conclusions and discussion

We have discussed two limitations that are present in the BGNF approach. The first results when the BGNF series is divergent, and may, at least when the system is integrable, be resolved by properly summing the series. The second arises when one tries to quantise the BGNF series or its summation, and is not resolvable. That is to say, given a BGNF series, there is no known method by which the correct energy spectrum may be obtained. Our recent work (paper II) on the quantum normal form (QNF) shows what one would expect the proper quantisation of the BGNF to yield. The QNF, which maintains the spirit of the BGNF, yields the BGNF series when the quantum operators are replaced by the corresponding classical variables. Also, the QNF series have, for the systems considered, yielded the same results as the RS series. Thus, although we know the correct quantum description of a system described in the BGNF approach, we do not know how to obtain that quantum description from the classical BGNF itself. As long as the quantisation problem is unresolved, the validity of the BGNF approach will be severely limited, irrespective of whether the BGNF series converges, diverges, or is summed.

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