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1984 J. Phys. A: Math. Gen. 17 109

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The algebraic quantisation of the Birkhoff–Gustavson normal form

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Received 12 November 1982, in final form 5 September 1983

Abstract. We develop an algebraic quantisation method for the Birkhoff–Gustavson normal form. For this purpose the Weyl quantisation rule is used. The method developed here for multidimensional systems allows one to calculate the energy levels and the transition probabilities. We give a brief review of the normal form, derive some of its general properties, and find a general analytic solution for the fourth-degree normal form for Hamiltonians of two degrees of freedom. In particular, this includes the Hénon–Heiles system. We compare the results of specific examples with other works. The question of canonically invariant quantisation, the relation to the quantum mechanical perturbation theory and the question of chaotic behaviour and quantum stochasticity are discussed. We show that the operators corresponding to the formal integrals of the motion are also quantum mechanical integrals. If the normal form accidentally terminates, so that the classical system is integrable, then this implies quantum integrability of the normal-form Hamiltonian.

1. Introduction

The main goal of this work is to provide an algebraic algorithm for the quantisation of the Birkhoff–Gustavson normal form for the Hamiltonians near an equilibrium point. This is made possible if quantum mechanical operators are assigned to the individual monomials of coordinates and momenta, by means of the Weyl quantisation rule. By virtue of the normal form the Hamilton operator thus obtained can be split into the sum, $\hat{H} = \hat{H}_0 + \hat{H}_A$, of the harmonic part \hat{H}_0 and anharmonic part \hat{H}_A , such that their commutator $[\hat{H}_0, \hat{H}_A]$ vanishes. Consequently, \hat{H}_0 and \hat{H}_A can be diagonalised simultaneously; in particular, \hat{H}_A is diagonal in a basis of harmonic functions. In the non-resonant case, where the (classical) normal form Hamiltonian depends only on the actions, the result reduces to the tori quantisation.

The quantisation of the normal form in resonant cases is reduced to simple algebraic manipulations involving diagonalisation of finite matrices. The calculation of the matrix elements of \hat{H}_A in the eigenspaces of \hat{H}_0 is simple as the operator \hat{H}_A can be expressed in terms of annihilation and creation operators. This purely algebraic method is easily programmable, and since its algorithm is straightforward, it might have advantages as compared with the tori quantisation, where the action integrals must be calculated numerically (cf Swimm and Delos 1979). The major novelty is that we are able to calculate transition probabilities. It should be noted that the quantisation of the normal form has already proved to be highly accurate (sometimes better than 1/100 of a percent) in various contexts (Swimm and Delos 1979, Reinhardt and Farelly 1982,

Williams and Koonin 1982) and is competing with perturbation theory, in particular for highly non-separable systems.

To show what is involved in the technique of this method we briefly explain the Birkhoff-Gustavson normal form, for the convenience of readers not familiar with it. Suppose we are studying the motion of a classical Hamilton system near an equilibrium point. The system may have an arbitrary number N of degrees of freedom. Then, to the lowest approximation the motion is described by N uncoupled (one-dimensional) harmonic oscillators. However, they become coupled if the higher-order (anharmonic) terms in the Taylor expansion of the potential are taken into account. As a result of the coupling the system becomes non-integrable in almost all cases; in fact, being a generic system, it is neither integrable nor ergodic but shows a stochastic transition at the critical energy (Berry 1983, Zaslavsky 1981, Robnik 1982a). Above the critical energy the motion is chaotic on the entire energy surface (in phase space), but below that energy it has all features of regular integrable motion. The numerical experiments (Hénon and Heiles 1964, Robnik 1981, 1982b) and the analytical investigations (Churchill *et al* 1978, Chang *et al* 1982, Braun 1973, Kummer 1976) show that there exist additional integrals of motion in that region of phase space. One can see them as invariant tori, i.e. as invariant curves of the Poincaré mappings of the surface of section. These are so dense on the energy surface that it is hard to resolve the gaps between them. For practical purposes the system is thus integrable in the regular region of phase space (i.e. below the critical energy of the stochastic transition).

We have then the difficult problem to predict analytically the invariant tori, or equivalently, to construct the integrals of motion. One of the possible methods is to calculate the normal form of the classical Hamiltonian. This was originally developed by Birkhoff for the non-resonant cases (no commensurability conditions for the frequencies of the harmonic oscillators), and consists of a series of canonical transformations, which are polynomial functions of coordinates and momenta. The algorithm is such that after $s-2$ transformations the new Hamiltonian is in normal form to degree s . By definition, this means that all monomials of order $\leq s$ in the power expansion of the Hamiltonian commute (Poisson brackets vanish) with the (unchanged) harmonic part of the Hamiltonian. In fact, all normal terms are just polynomials of the N actions. This formal procedure can be extended ad infinitum ($s \rightarrow \infty$), whereby one obtains a power expansion of the Hamiltonian as a function of the actions. Each of N actions, when expressed in terms of the original coordinates and momenta, is itself a power expansion of an integral of motion. However, Siegel (1941) has proved that the series diverges, which is related to the non-integrability of the Hamiltonian: if the convergence radius of the series were non-zero, then the system would be rigorously integrable in some region of phase space, since the integrals of motion would be analytic there. But according to the KAM theorem a generic system is non-integrable, and we have thin gaps of irregular, chaotic motion between the invariant tori unless the system is accidentally rigorously integrable. The convergence radius of such series can generally never be made non-zero, whatever the method we use. Hence the name formal integral of motion.

Birkhoff's algorithm has been generalised by Gustavson (1966) to the resonant cases. (See also Arnold 1980.) The divergence difficulties of course still exist. But one should observe that while the infinite series has no rigorous meaning, the Hamiltonian in normal form truncated after the degree s is a rigorously integrable system, which is close to the original system in 'some sense'. It has never been clarified how this 'closeness' should be measured, but numerical and analytical experience show a

remarkable accuracy of the approximation of periodic orbits, invariant tori and their bifurcations. It has been taken for granted that the truncated normal form becomes exact asymptotically as we approach the equilibrium point. Clearly, above the critical energy, where the stochastic transition (onset of irregular, chaotic motion) occurs, these formal integrals of motion lose their meaning completely, as the large scale invariant tori no longer exist.

Assuming that the truncated normal form is a sufficiently good approximation of the original Hamiltonian, we can immediately find the corresponding Hamilton operator $\hat{H} = \hat{H}_0 + \hat{H}_A$, by applying the Weyl quantisation (de Groot and Suttorp 1972) to it. This formal procedure might appear *ad hoc* at first sight, since the question of commutation of quantisation and classical canonical transformations is a generally unsolved problem. We shall return to this question in § 6, but it should be noted that according to experience the result of quantisation of the normal form is remarkably close to the predictions of quantum perturbation theory. We show this for an example in § 7. In § 6 we shall also consider the problem of the canonically covariant quantisation and the problems related to the quantum integrability. We show that under certain conditions the classical integrals of the normal form are also quantum integrals.

2. The Birkhoff–Gustavson normal form

In this section we briefly review the algorithm leading to the Birkhoff–Gustavson normal form, which is necessary to make the present work selfcontained, and allows us to derive some properties of the normal form (see Gustavson (1966); a review is given in Swimm and Delos (1979)). In § 3 we give some properties of the normal form, such as: (1) the normal form is always an even function of momenta; (2) in equation (26) we give the most general expression for the normal form; (3) in case $N = 2$ we give the system of basic variables and calculate their Poisson brackets. The reader familiar with Gustavson’s work can skip this section.

Consider a Hamiltonian with N degrees of freedom in the form

$$H(x, y) = \sum_{j=2}^{\infty} H^{(j)}(x, y), \tag{1}$$

where $x := (x_1, x_2, \dots, x_N)$ are the coordinates, $y := (y_1, y_2, \dots, y_N)$ the momenta, and

$$H_0(x, y) := H^{(2)}(x, y) = \sum_{k=1}^N \frac{\omega_k}{2} (x_k^2 + y_k^2) \tag{2}$$

is the harmonic part of (1), with ω_k , $1 \leq k \leq N$, being the oscillation frequencies. Each term $H^{(j)}$ in (1) is assumed to be a homogeneous polynomial of degree j , i.e.

$$H^{(j)}(x, y) = \sum_{k:|l|=j} h_{kl} x^k y^l, \tag{3}$$

where h_{kl} are real constants, and we use multi-indices like $k := (k_1, k_2, \dots, k_N)$ with the definitions

$$|k| := |k_1| + |k_2| + \dots + |k_N|, \quad x^k := x_1^{k_1} x_2^{k_2} \dots x_N^{k_N}.$$

We say that there is an *r*th-fold resonance at the equilibrium point $(x, y) = (0, 0)$, if there are *r* linearly independent commensurability conditions between the frequencies, i.e.

$$\sum_{k=1}^N a_{ik} \omega_k = 0, \quad (4)$$

where $i = 1, 2, \dots, r$, and the rank of the real matrix a_{ik} equals *r*. The equilibrium point is said to be non-resonant if there are no rational connections (4).

We now define the normal form. The Hamiltonian (1) is in normal form to degree *s* if

$$D_{(x,y)} H^{(j)}(x, y) = 0, \quad (5)$$

for $2 \leq j \leq s$, where the partial differential operator

$$D_{(x,y)} := \{H_0, \cdot\} = \sum_{k=1}^N \omega_k \left(x_k \frac{\partial}{\partial y_k} - y_k \frac{\partial}{\partial x_k} \right), \quad (6)$$

so that (5) is just the Poisson bracket $\{H_0, H^{(j)}\}$.

It is useful to introduce the quantities

$$\tau_k := \frac{1}{2}(x_k^2 + y_k^2), \quad 1 \leq k \leq N. \quad (7)$$

The following theorem is the main result of Gustavson (1966).

Theorem (Gustavson). If the Hamiltonian (1) is in normal form to all orders ($s = \infty$), and is represented by a formal series, then:

(a) For an *r*th-fold resonance we have $N - r$ independent formal integrals of the motion,

$$I_1 = \sum_{k=1}^N \mu_{lk} \tau_k, \quad (8)$$

where μ_{lk} , $1 \leq l \leq N - r$, are the independent solutions of the commensurability conditions (4), i.e.

$$\sum_{k=1}^N a_{ik} \mu_{lk} = 0, \quad 1 \leq i \leq r.$$

In this case the Hamiltonian (1) is itself an integral independent of I_k 's.

(b) In the non-resonant case we have N independent integrals $\tau_1, \tau_2, \dots, \tau_N$, and the Hamiltonian (1) becomes a function of them, i.e.

$$H = H(\tau_1, \tau_2, \dots, \tau_N). \quad (9)$$

Given a Hamilton system with the quadratic kinetic energy + potential energy, we can always shift the energy scale, shift and rotate the coordinate axes x_k , and stretch the coordinates and momenta in such a way that the Hamiltonian appears in the form

$$H(x, y) = H_0 + \sum_{j=3}^{\infty} U^{(j)}(x), \quad (10)$$

where

$$H_0 = \sum_{k=1}^N \omega_k \tau_k$$

is the harmonic part, while $U^{(j)}(x)$ are just the homogeneous polynomials of degree j arising from the Taylor expansion of the potential $U = U(x)$ around the equilibrium point $x = 0$. The Hamiltonian (10) is thus a special case of (1): the anharmonic terms depend only on the coordinates x . Note that (10) is an even function of momenta.

The question now is whether the Hamiltonian (10) can be brought to the normal form by a canonical transformation $(x, y) \rightarrow (q, p)$, so that $H(x, y) \rightarrow \tilde{H}(q, p)$, where $q = (q_1, \dots, q_N)$, $p = (p_1, \dots, p_N)$ are new coordinates and momenta, respectively, and $\tilde{H}(q, p)$ is the normal form Hamiltonian. The answer is positive by theorem 1 in Gustavson's work.

Let $H(x, y)$ from (1) be in normal form to degree $s-1$. Then there exists a generating function

$$G^{(s)}(x, p) = xp + W^{(s)}(x, p), \tag{11}$$

where $W^{(s)}(x, p)$ is a homogeneous polynomial of degree s , such that after the canonical transformation

$$q = x + \partial W^{(s)}(x, p) / \partial p, \quad y = p + \partial W^{(s)}(x, p) / \partial x, \tag{12}$$

the new Hamiltonian $\tilde{H}(q, p)$ is in normal form up to degree s . To show this consider first the equality

$$H(x, p + \partial W^{(s)} / \partial x) = \tilde{H}(x + \partial W^{(s)} / \partial p, p). \tag{13}$$

From the power expansion of these expressions we see

$$H^{(j)}(\xi, \eta) = \tilde{H}^{(j)}(\xi, \eta), \quad 2 \leq j \leq s-1, \tag{14}$$

where (ξ, η) stand for the arguments of the functions. In other words, those terms which are already in normal form are not affected by the transformation. The homogeneous polynomial $W^{(s)}(x, p)$ determining the generating function can be so chosen that

$$\{H_0, \tilde{H}^{(s)}\} = D_{(q,p)} \tilde{H}^{(s)}(q, p) = 0,$$

i.e. that \tilde{H} is in normal form up to degree s . This can be seen by equating terms of order s in (13), whence

$$D_{(x,p)} W^{(s)}(x, p) = H^{(s)}(x, p) - \tilde{H}^{(s)}(x, p). \tag{15}$$

By definition $\tilde{H}^{(s)}$ must be in the kernel of the partial differential operator $D_{(x,p)}$. Now, since D is a linear operator, it allows a unique decomposition of the space of polynomials into a direct sum of the kernel N and the range R . Accordingly, each polynomial can be uniquely decomposed into a sum of its N component and R component. To solve (15) we take $\tilde{H}^{(s)}$ to be the N component of $H^{(s)}$. The solution for $W^{(s)}$ in (15) is then determined up to an arbitrary additive polynomial from N . To make $W^{(s)}$ unique we require, following Gustavson, that $W^{(s)}$ is in the range R of D .

Having obtained the solution for $\tilde{H}^{(s)}$ and $W^{(s)}$ we can calculate the remaining terms of the new Hamiltonian \tilde{H} in the power expansion of (13). It turns out that for each $i = 2, 3, 4, \dots$

$$\tilde{H}_{(x,p)}^{(i)} = H_{(x,p)}^{(i)} + \sum_{j!} \frac{1}{j!} \left[\frac{\partial^j H^{(i+1)}}{\partial p^j} \left(\frac{\partial W^{(s)}}{\partial x} \right)^j - \frac{\partial^j \tilde{H}^{(i+1)}}{\partial x^j} \left(\frac{\partial W^{(s)}}{\partial p} \right)^j \right], \tag{16}$$

where the summation over j is restricted by the conditions

$$l + |j|(s-2) = i, \quad l \leq |j| \leq 1 < i, \quad l \geq 2, s \geq 3,$$

and we use the multi-index notations

$$j! := j_1! j_2! \dots j_N!, \quad \partial^{|j|} H^{(l)} / \partial p^j := \partial^{|j|} H^{(l)}(x, p) / \partial p_1^{j_1} \partial p_2^{j_2} \dots \partial p_N^{j_N}, \\ (\partial W^{(s)} / \partial x)^j := (\partial W^{(s)} / \partial x_1)^{j_1} \dots (\partial W^{(s)} / \partial x_N)^{j_N}.$$

One can see that for $i < s$ we get indeed (14), while for $i = s$ we recover equation (15). All terms $\tilde{H}^{(j)}$, $j > s$, can be then calculated successively by the formula (16).

By assumption $H^{(2)}(x, y)$ is already in normal form. Consequently, by a series of successive canonical transformations generated by $G^{(3)}, G^{(4)}, \dots, G^{(s)}, \dots$ we can calculate the normal form to an arbitrary degree.

3. The structure of the normal form

The fact that the normal form can *always* be represented as in (26) is the main result of the classical part of our paper.

We now prove the following property of the canonical transformation (11)–(16).

Proposition. If the Hamiltonian (1) is an even function of momenta, i.e. $H(x, y) = H(x, -y)$, and is assumed in normal form up to degree $s-1$, then the Hamiltonian $\tilde{H}(q, p)$ obtained according to the transformation (11)–(16) is also an even function of momenta, i.e.

$$\tilde{H}(q, p) = \tilde{H}(q, -p).$$

Proof. If $H(x, y)$ is even in momenta, then $H^{(s)}(x, y)$ is too, and *a fortiori* its N component $\tilde{H}^{(s)}$. The RHS of (15) is thus even. Since the operator D switches the parity, this implies that $W^{(s)}$ is an odd function of momenta, i.e. $W^{(s)}(x, p) = -W^{(s)}(x, -p)$. But then for $|j|$ even or odd the factors in the two products in the bracket under the summation symbol of (16) have the parity $(+, +; +, +)$ and $(-, -; +, +)$, respectively. Consequently, each term $\tilde{H}^{(j)}$ of the new Hamiltonian is also an even function of momenta.

For the Hamiltonian system (10), which has the usual form kinetic energy + potential energy, we have the result that its normal form to any degree s is an even function of momenta. This will be used later on.

Note that odd parity in momentum variables is *not* invariant against the canonical transformation (11)–(16). Precisely analogous results apply to the parity in coordinates: even parity is preserved, but odd parity is not invariant under the canonical transformations.

In order to study the structure of the general normal form we now make a *non-canonical* transformation to the *complex* variables

$$z_k := (1/\sqrt{2})(x_k + iy_k), \quad 1 \leq k \leq N, \quad (17)$$

so that the coordinates and momenta are

$$x_k = (1/\sqrt{2})(z_k + z_k^*), \quad y_k = (1/i\sqrt{2})(z_k - z_k^*), \quad (18)$$

where z_k^* is the complex conjugate of z_k . We see from (7) that $\tau_k = z_k z_k^*$, and with

$\theta_k := \arg z_k$, we obtain

$$z_k = \sqrt{\tau_k} e^{i\theta_k}, \quad 1 \leq k \leq N. \quad (19)$$

It can be easily seen that the operator $D_{(x,y)}$ from (6) becomes

$$D = \sum_{k=1}^N \omega_k \frac{\partial}{\partial \theta_k}. \quad (20)$$

By definition the normal form (1) contains only polynomials from the kernel N of the operator D . A basis of N can be most easily determined by using the complex variables (17). Inserting (18) into the normal form (1) yields a power series in complex variables z_k, z_k^* . But since (10) is an even function of momenta, so is its normal form (1), and all coefficients in the series are real. Since the series $H(x, y)$ is real valued we conclude that if $z^m z^{*n}$ occurs in the formal series, then its complex conjugate $z^{*m} z^n$ must do so with the same real coefficient. Here we used again the multi-index notation $z = (z_1, z_2, \dots, z_N)$, $m = (m_1, m_2, \dots, m_N)$, etc.

The monomials $z^m z^{*n}$ in the kernel N of the operator D given in (20) are determined by

$$Dz^m z^{*n} = 0,$$

whence

$$\omega(m - n) = \sum_{k=1}^N \omega_k (m_k - n_k) = 0. \quad (21)$$

This condition implies that $m_k - n_k$, $1 \leq k \leq N$, must be a linear combination of the rows of the commensurability matrix a_{lk} , $1 \leq l \leq r$, given in (4). To simplify the expressions we assume that each row vector $(a_{l1}, \dots, a_{lN}) = \alpha_l$ has integer components without a common factor. From (21) we obtain

$$m - n = \sum_{l=1}^r \gamma_l \alpha_l, \quad (22)$$

where γ_l are non-negative numbers. Note that the integer vectors α_l can have negative components. It is not very convenient to write

$$z^m z^{*n} = \tau^n z^{\sum_{l=1}^r \gamma_l \alpha_l}$$

because negative powers of z can appear in the second factor. Instead, we introduce the resonant monomials

$$K_l := \tau^{|\alpha_l|/2} \exp\left(i \sum_{k=1}^N a_{lk} \theta_k\right) = u_1^{|\alpha_{l1}|} u_2^{|\alpha_{l2}|} \dots u_N^{|\alpha_{lN}|}, \quad (23)$$

where

$$u_k = \begin{cases} z_k, & \text{if } a_{lk} \geq 0, \\ z_k^*, & \text{if } a_{lk} < 0. \end{cases} \quad (24)$$

It can be easily seen that $DK_l = 0$, i.e. K_l , $1 \leq l \leq r$, are constants of the motion of the harmonic part $H_0 = \sum_{k=1}^N \omega_k \tau_k$. Writing

$$\gamma := (\gamma_1, \dots, \gamma_r) \quad \text{and} \quad K := (K_1, \dots, K_r), \quad (25)$$

we obtain the most general expression

$$H(x, y) = \sum_{\gamma} f_{\gamma}(\tau)(K^{\gamma} + K^{*\gamma}) \quad (26)$$

for the normal form (1), where $f_{\gamma}(\tau)$ is a real polynomial. The summation runs over all non-negative integers $\gamma = (\gamma_1, \dots, \gamma_r)$ and $K^{\gamma} = K_1^{\gamma_1} K_2^{\gamma_2} \dots K_r^{\gamma_r}$ etc. We see that the normal form is generally a function of the variables $\tau = (\tau_1, \tau_2, \dots, \tau_N)$ defined in (7) and $K = (K_1, K_2, \dots, K_r)$, as defined in (23)–(25). In the non-resonant case $r = 0$ and H depends only on τ , which are thus action variables.

We shall call $\{H_0, \tau, K, K^*\}$ the set of basic variables since the normal form can be expressed as a function of them. By definition each basic variable commutes with H_0 (Poisson bracket vanishes). It can be shown that they form a closed system in the sense that the Poisson bracket for any pair is a polynomial of basic variables. The Poisson brackets can be easily calculated by using the expressions

$$\{z_k^*, z_l\}_{(x,y)} = i\delta_{kl}, \quad \{z_k, z_l\}_{(x,y)} = \{z_k, z_l\}_{(x,y)} = 0. \quad (27)$$

Let us specialise to two degrees of freedom, $N = 2$, assuming $r = 1$, $\alpha_1 = (a_{11}, a_{12}) = (t_2, -t_1)$, i.e. $\omega_1/\omega_2 = t_1/t_2$. Then the Poisson brackets of $\{H_0, \tau_1, \tau_2, K, K^*\}$ read

$$\begin{aligned} \{\tau_1, K\} &= it_2 K, & \{\tau_1, K^*\} &= -it_2 K^*, \\ \{\tau_2, K\} &= -it_1 K, & \{\tau_2, K^*\} &= +it_1 K^*, \\ \{K, K^*\} &= i\tau_1^{t_2-1} \tau_2^{t_1-1} (t_1^2 \tau_1 - t_2^2 \tau_2), \\ \{H_0, \tau_1\} &= \{H_0, \tau_2\} = \{H_0, K\} = \{H_0, K^*\} = \{\tau_1, \tau_2\} = 0. \end{aligned} \quad (28)$$

The normal form (26) equals ($\gamma \equiv \gamma_1$)

$$H(x, y) = \sum_{\gamma=0}^{\infty} f_{\gamma}(\tau_1, \tau_2)(K^{\gamma} + K^{*\gamma}), \quad (29)$$

from which we can derive an additional property: in the case of an even order resonance, i.e. $|t_1| + |t_2| = \text{even integer}$, τ_1, τ_2, K are monomials of even order in variables x, y . Consequently, for an even order resonance, such as $\omega_1/\omega_2 = 1$, or $\omega_1/\omega_2 = \frac{1}{3}$, the normal form $H(x, y)$ in (1) contains only even order terms, i.e. $H^{(j)}(x, y) = 0$ if j is odd.

4. Some examples

In this section we calculate the general normal form up to degree 4 for systems with two degrees of freedom, $N = 2$. The non-resonant case is considered first, and then we treat the case of the lowest-order resonance $\omega_1/\omega_2 = 1$. In both cases we give explicit results for two special potentials, one of them being the Hénon–Heiles potential (1964).

A warning is in order here: while the examples in this section are still calculable by hand, the higher-order normal forms are not. Even for $N = 2$ the calculation of the eighth-degree normal form involves polynomials of order 495 and 495×495 matrices must be inverted. For this reason one uses a computer for symbolic algebraic manipulations. This procedure is usually still partially numerical (cf Gustavson 1966, Swimm and Delos 1979), but we have done completely symbolic calculations using the REDUCE programming language (Schrüfer and Robnik 1983). The examples of this section were used to test the computer routines.

We assume the Hamiltonian (10) in the form

$$\begin{aligned} H &= \omega_1 \tau_1 + \omega_2 \tau_2 + U^{(3)}(x_1, x_2) + U^{(4)}(x_1, x_2), \\ U^{(3)} &= ax_1^3 + bx_1^2 x_2 + cx_1 x_2^2 + dx_2^3, \\ U^{(4)} &= Ax_1^4 + Bx_1^3 x_2 + Cx_1^2 x_2^2 + Dx_1 x_2^3 + Ex_2^4, \end{aligned} \quad (30)$$

where $\omega_1/\omega_2 \neq \frac{1}{2}, 2$. First we calculate the polynomial,

$$W^{(3)}(x_1, x_2, p_1, p_2) = \sum_{k+l+m+n=3} W(klmn) x_1^k x_2^l p_1^m p_2^n, \quad (31)$$

whose coefficients are determined by (15). Now, since $\tilde{H}^{(3)}_{(x,p)} = 0$, we have to solve

$$D_{(x,p)} W^{(3)} = U^{(3)}. \quad (32)$$

After a straightforward and lengthy calculation we obtain the coefficients

$$\begin{aligned} W(0030) &= 2a/3\omega_1 = v_1, & W(0003) &= 2d/3\omega_2 = v_2, \\ W(1110) &= b/2\omega_1(1 - \omega_2^2/4\omega_1^2) =: M = v_3, \\ W(1101) &= c/2\omega_2(1 - \omega_1^2/4\omega_2^2) =: N = v_4, \\ W(2010) &= a/\omega_1 = v_5, & W(0201) &= d/\omega_2 = v_6, \\ W(2001) &= (\omega_1/\omega_2 - \omega_2/2\omega_1)M = v_7, & W(0210) &= (\omega_2/\omega_1 - \omega_1/2\omega_2)N = v_8, \\ W(0021) &= \omega_1 M/\omega_2 = v_9, & W(0012) &= \omega_2 N/\omega_1 = v_{10}, \end{aligned} \quad (33)$$

while all other coefficients vanish (ten of total 20 coefficients).

The next step is now to calculate $\tilde{H}^{(4)}(x, p)$. Using (16),

$$\tilde{H}^{(4)}(x, p) = H^{(4)}(x, p) + \frac{\omega_1}{2} \left[\left(\frac{\partial W^{(3)}}{\partial x_1} \right)^2 - \left(\frac{\partial W^{(3)}}{\partial p_1} \right)^2 \right] + \frac{\omega_2}{2} \left[\left(\frac{\partial W^{(3)}}{\partial x_2} \right)^2 - \left(\frac{\partial W^{(3)}}{\partial p_2} \right)^2 \right], \quad (34)$$

we obtain the coefficients $h(klmn)$ of

$$\tilde{H}^{(4)}(x, y) = \sum_{k+l+m+n=4} h(klmn) x_1^k x_2^l y_1^m y_2^n, \quad (35)$$

listed in table 1. There are 19 non-zero and 16 vanishing coefficients. Having done this the fourth-degree normal form $\tilde{H}^{(4)}(x, y)$ is equal to the N component of (35).

We shall write the normal form as in the standard expression (29), i.e.

$$H = \omega_1 \tau_1 + \omega_2 \tau_2 + g_{20} \tau_1^2 + g_{11} \tau_1 \tau_2 + g_{02} \tau_2^2 + (\gamma_1 \tau_1 + \gamma_2 \tau_2)(K + K^*) + \gamma_3(K^2 + K^{*2}), \quad (36)$$

where

$$K = z_1 z_2^* = \frac{1}{2}[(x_1 x_2 + p_1 p_2) + i(x_2 p_1 - x_1 p_2)] \quad (37)$$

so that

$$K + K^* = x_1 x_2 + p_1 p_2, \quad K^2 + K^{*2} = \frac{1}{2}[(x_1 x_2 + p_1 p_2)^2 - (x_2 p_1 - x_1 p_2)^2]. \quad (38)$$

The $\omega_1/\omega_2 = 1$ resonance is the only one affecting the fourth-order normal form. ($\omega_1/\omega_2 = \frac{1}{2}, 2$ has been excluded by assumption. This would change already the third-order normal form.) In this case γ_1, γ_2 and γ_3 (which should not be confused with the summation index γ in (29)) have to be determined with $\omega_1 = \omega_2 = \omega$, while

Table 1. The non-zero coefficients $h(klmn)$.

$$\begin{aligned}
h(4000) &= A - \frac{1}{2}(\omega_1 v_5^2 + \omega_2 v_7^2) \\
h(0400) &= -\frac{1}{2}(\omega_1 v_8^2 + \omega_2 v_6^2) \\
h(0040) &= -\frac{1}{2}(9\omega_1 v_1^2 + \omega_2 v_9^2) \\
h(0004) &= E - \frac{1}{2}(\omega_1 v_{10}^2 + 9\omega_2 v_2^2) \\
h(3100) &= B - (\omega_1 v_3 v_5 + \omega_2 v_4 v_7) \\
h(0031) &= -(6\omega_1 v_1 v_9 + 2\omega_2 v_9 v_{10}) \\
h(0013) &= -2(\omega_1 v_9 v_{10} + 3\omega_2 v_2 v_{10}) \\
h(1300) &= D - (\omega_1 v_3 v_8 + \omega_2 v_4 v_6) \\
h(2200) &= C - \frac{1}{2}(\omega_1 v_3^2 + 2\omega_1 v_5 v_8 + \omega_2 v_4^2 + 2\omega_2 v_7 v_6) \\
h(2020) &= \frac{1}{2}(4\omega_1 v_5^2 + \omega_2 v_3^2 - 6\omega_1 v_1 v_5 - 2\omega_2 v_7 v_9) \\
h(2002) &= \frac{1}{2}(4\omega_1 v_7^2 + \omega_2 v_4^2 - 2\omega_1 v_5 v_{10} - 6\omega_2 v_2 v_7) \\
h(0220) &= \frac{1}{2}(\omega_1 v_3^2 + 4\omega_2 v_8^2 - 6\omega_1 v_1 v_8 - 2\omega_2 v_6 v_9) \\
h(0202) &= \frac{1}{2}(\omega_1 v_4^2 + 4\omega_2 v_6^2 - 2\omega_1 v_8 v_{10} - 6\omega_2 v_2 v_6) \\
h(0022) &= -(2\omega_1 v_9^2 + 3\omega_1 v_1 v_{10} + 2\omega_2 v_{10}^2 + 3\omega_2 v_2 v_9) \\
h(2011) &= 4\omega_1 v_5 v_7 + \omega_2 v_3 v_4 - 2\omega_1 v_5 v_9 - 2\omega_2 v_7 v_{10} \\
h(1102) &= 2\omega_1 v_4 v_7 + 2\omega_2 v_4 v_6 - \omega_1 v_3 v_{10} - 3\omega_2 v_2 v_4 \\
h(1120) &= 2\omega_1 v_3 v_5 + 2\omega_2 v_3 v_8 - 3\omega_1 v_1 v_3 - \omega_2 v_4 v_9 \\
h(0211) &= \omega_1 v_3 v_4 + 4\omega_2 v_8 v_6 - 2\omega_1 v_8 v_9 - 2\omega_2 v_6 v_{10} \\
h(1111) &= 2\omega_1 v_3 v_7 + 2\omega_1 v_4 v_5 + 2\omega_2 v_3 v_6 + 2\omega_2 v_4 v_8 - 2\omega_1 v_3 v_9 - 2\omega_2 v_4 v_{10}.
\end{aligned}$$

in all other cases $\gamma_3 = \gamma_2 = \gamma_1 = 0$. The easiest way of finding the coefficients of normal form (36) is to use the complex variables. We distinguish between two cases.

(a) *The non-resonant case and higher-order resonances* ($\omega_1/\omega_2 \neq \frac{1}{2}, 2, 1$)

The result is

$$\begin{aligned}
g_{20} &= \frac{3}{2}h(4000) + \frac{1}{2}h(2020) + \frac{3}{2}h(0040), \\
g_{11} &= h(2200) + h(2002) + h(0220) + h(0022), \\
g_{02} &= \frac{3}{2}h(0400) + \frac{1}{2}h(0202) + \frac{3}{2}h(0004), \quad \gamma_1 = \gamma_2 = \gamma_3 = 0.
\end{aligned} \tag{39}$$

(b) *The lowest-order resonance*, $\omega_1 = \omega_2$

The coefficients g_{20} , g_{11} , g_{02} are as in (39), while

$$\begin{aligned}
\gamma_1 &= \frac{3}{4}h(3100) + \frac{3}{4}h(0031) + \frac{1}{4}h(2011) + \frac{1}{4}h(1120), \\
\gamma_2 &= \frac{3}{4}h(1300) + \frac{3}{4}h(0013) + \frac{1}{4}h(1102) + \frac{1}{4}h(0211), \\
\gamma_3 &= \frac{1}{4}h(2200) - \frac{1}{4}h(2002) - \frac{1}{4}h(0220) + \frac{1}{4}h(0022) + \frac{1}{4}h(1111).
\end{aligned} \tag{40}$$

However, we choose $\omega_1 = \omega_2 = 1$ without loss of generality. The coefficients v_1, v_2, \dots, v_{10} in (33) simplify considerably and we obtain the coefficients $h(klmn)$ given in table 2. With this result we can write (39) and (40) explicitly in terms of the original potential (i.e. its Taylor coefficients) in (30),

$$\begin{aligned}
g_{20} &= \frac{3}{2}(A - \frac{5}{2}a^2 - \frac{5}{18}b^2), & g_{11} &= C - \frac{2}{3}(b^2 + c^2) - 3(ac + bd), \\
g_{02} &= \frac{3}{2}(E - \frac{5}{2}d^2 - \frac{5}{18}c^2), & \gamma_1 &= \frac{3}{4}(B - \frac{10}{3}b(a + \frac{1}{3}c)), \\
\gamma_2 &= \frac{3}{4}(D - \frac{10}{3}c(d + \frac{1}{3}b)), & \gamma_3 &= \frac{1}{4}(C - 2(b^2 + c^2) + ac + bd).
\end{aligned} \tag{41}$$

The formulae (39)–(41) are general. It is useful to consider two specific systems, which will be used also in subsequent sections, where the quantisation is studied.

Table 2. The coefficients of table 1 when $\omega_1 = \omega_2 = 1$.

$h(4000) = A - \frac{1}{2}(a^2 + \frac{1}{3}b^2)$	$h(2002) = \frac{2}{3}(b^2 + c^2 - 3ac - 3bd)$
$h(0400) = -\frac{1}{2}(\frac{1}{3}c^2 + d^2)$	$h(0220) = \frac{2}{3}(b^2 + c^2 - 3ac - 3bd) = h(2002)$
$h(0040) = -2(a^2 + \frac{1}{3}b^2)$	$h(0202) = 0$
$h(0004) = E - 2(\frac{1}{3}c^2 + d^2)$	$h(0022) = -\frac{4}{3}(2b^2 + 2c^2 + 3ac + 3bd)$
$h(3100) = B - \frac{2}{3}b(a + \frac{1}{3}c)$	$h(2011) = 0$
$h(0031) = -\frac{8}{3}b(a + \frac{1}{3}c)$	$h(1102) = 0$
$h(0013) = -\frac{8}{3}c(\frac{1}{3}b + d)$	$h(1120) = 0$
$h(1300) = D - \frac{2}{3}c(\frac{1}{3}b + d)$	$h(0211) = 0$
$h(2200) = C - \frac{1}{3}(2b^2 + 2c^2 + 3ac + 3bd)$	$h(1111) = -\frac{4}{3}(b^2 + c^2 - 3ac - 3bd) = -2h(2002)$
$h(2020) = 0$	

Example 1. ($\omega_1/\omega_2 \neq 1/2, 2, 1$)

Let c and C be non-zero, while all other coefficients of $U^{(3)}$ and $U^{(4)}$ in (30) vanish. The normal form up to the fourth degree according to (39) reads

$$H = \omega_1 \tau_1 + \omega_2 \tau_2 + \tau_1 \tau_2 \left(C + \frac{2\omega_2 c^2}{\omega_1^2 - 4\omega_2^2} \right) - \frac{c^2 \tau_2^2}{4\omega_1} \frac{3\omega_1^2 - 8\omega_2^2}{\omega_1^2 - 4\omega_2^2}. \quad (42)$$

Example 2. ($\omega_1 = \omega_2 = 1$):

We take the Hénon–Heiles system (1964) $b = \lambda, d = \lambda \eta$ (all other coefficients of $U^{(3)}$ and $U^{(4)}$ vanish) as an example of a resonant case (see also Gustavson 1966, Swimm and Delos 1979). The result follows directly from (41),

$$\begin{aligned} g_{20} &= -\frac{5}{12}\lambda^2, & g_{11} &= -\frac{2}{3}\lambda^2(1 + \frac{9}{2}\eta), & g_{02} &= -\frac{15}{4}\lambda^2\eta^2, \\ \gamma_1 &= \gamma_2 = 0, & \gamma_3 &= -\frac{1}{2}\lambda^2(1 - \frac{1}{2}\eta), \end{aligned} \quad (43)$$

i.e. the normal form up to degree 4 of the Hénon–Heiles system reads:

$$\begin{aligned} H(x, y) &= \frac{1}{2}(x_1^2 + y_1^2) + \frac{1}{2}(x_2^2 + y_2^2) - \lambda^2 \left\{ \frac{5}{12} [\frac{1}{2}(x_1^2 + y_1^2)]^2 + (\frac{2}{3} + 3\eta) [\frac{1}{4}(x_1^2 + y_1^2)(x_2^2 + y_2^2)] \right. \\ &\quad \left. + \frac{15}{4} \eta^2 [\frac{1}{2}(x_2^2 + y_2^2)]^2 + \frac{1}{4}(1 - \frac{1}{2}\eta) [(x_1 x_2 + y_1 y_2)^2 - (x_2 y_1 - x_1 y_2)^2] \right\}. \end{aligned} \quad (44)$$

In the special case $\lambda = 1, \eta = -\frac{1}{3}$ we have a complete agreement with the coefficients in Gustavson’s numerical example (1966). (As can be verified, the fourth-degree coefficients from Gustavson’s table II are exactly reproduced.) However, comparison with the example by Swimm and Delos (1979), where $\lambda = 0.0125$ and $\eta = -\frac{1}{3}$, shows that their coefficients $g_{20}, g_{11}, g_{02}, \gamma_3$ as given in their equation (29) are correct if divided by a factor 8. In other words, their equation (29) refers to $\lambda = \sqrt{2}/40$ rather than to $\lambda = 1/80$. Similarly, the coefficients of their fourth-degree normal form $\Gamma^{(4)}$ as given in their equation (33b) are correct if divided by a factor 80, i.e. they actually refer to $\lambda = 1/\sqrt{80}$ but not to $\lambda = 1/80$ as they claimed there.

5. The algebraic quantisation of the normal form

The philosophy of the quantisation method presented in this work is simple: suppose the normal form (1) of a given system (10) is known, and assume (non-trivially) that the quantum operators corresponding to the coordinates x and momenta y satisfy the

canonical commutation relations, i.e.

$$[\hat{x}_k, \hat{y}_l] = i\hbar \delta_{kl}. \quad (45)$$

Then one has to determine the Hamilton operator $\hat{H} = \hat{H}_0 + \hat{H}_A$ corresponding to the normal form, and finally to find its energy eigenvalues.

To quantise the normal form means that we must assign an operator to the normal Hamiltonian. Because the normal form is written as a formal series of (multi-dimensional) monomials, this procedure is feasible only if the quantisation scheme is linear. In other words, the map $\hat{W}: f \rightarrow \hat{f}$, where f is a classical phase space function and \hat{f} is the corresponding Hermitian operator, should be linear, i.e. $\hat{W}(af + bg) = a\hat{f} + b\hat{g}$. There are a number of different linear quantisation schemes, e.g. the Weyl rule, the Born–Jordan rule, the symmetrisation rule, etc. Although it might be argued that Weyl’s rule is the ‘best’ (Springborg 1983), this does not remove the fundamental difficulty. Namely, the fact remains that there does *not* exist a linear quantisation map \hat{W} which preserves the Poisson structure. (See Abraham and Marsden 1978, Castellani 1978 and references therein.) This implies that no linear quantisation can be canonically covariant. The property (45) holds only in special coordinate systems in phase space, and changes with the (general) canonical transformations of these coordinates. Strictly speaking, we do not know in which system (45) holds, but it can be argued that this is the case at least when the Hamiltonian is in the usual form ‘quadratic kinetic energy + potential energy’. Our assumption that (45) is satisfied for the normal form is thus indeed non-trivial and must be regarded as a working hypothesis.

We describe now our quantisation method. To begin with let us recall that the normal form $H(x, y) = H_0(x, y) + H_A(x, y)$, where

$$H_A(x, y) = \sum_{j=3}^{\infty} H^{(j)}(x, y) \quad (46)$$

is its anharmonic part, is an infinite sum of multidimensional monomials in coordinates and momenta, i.e.

$$H = \sum_{\text{mon}} h(\text{mon}) x^k y^l, \quad (47)$$

where $k = (k_1, \dots, k_N)$ and $l = (l_1, \dots, l_N)$ are non-negative integers. The problem $\hat{W}: H \rightarrow \hat{H}$ will be solved if we determine the operators corresponding to each of the monomials in (47). We assume that \hat{W} is the Weyl correspondence rule (see the useful study of this in the book by de Groot and Suttorp (1972)). The following comments are essential for subsequent developments.

(C1) Contrary to a claim by Korsch (1982) \hat{W} does *not* preserve the commutation, in general (cf Hietarinta 1982). Thus if the Poisson bracket $\{f, g\}$ vanishes, then the quantum commutator $[\hat{W}(f), \hat{W}(g)] = [\hat{f}, \hat{g}]$ does not vanish, in general. *Example:* $f = qp^2$, $g = q^2p^4 = f^2$, so that $\{f, g\} = 0$. It can be shown by using either the general definition of \hat{W} involving the Moyal brackets, or by the algebraic rule for polynomials (see below) that $[\hat{f}, \hat{g}] = -2i\hbar^3 \hat{p}^3 \neq 0$.

(C2) \hat{W} does *not* satisfy the so-called squaring axiom (Wan and McKenna 1982). Thus in general $\hat{W}(f^2) \neq \hat{f}^2$. This can be inferred from the above example: if \hat{g} were equal to \hat{f}^2 then the commutator $[\hat{f}, \hat{g}]$ would vanish. Moreover, even if f and g are such that $\{f, g\} = 0$ and *accidentally* also $[\hat{f}, \hat{g}] = 0$, then $g = f^2$ does not imply $\hat{g} = \hat{f}^2$. *Example:* $f = qp$, $g = f^2 = q^2p^2$ and $\hat{f} = \hat{q}\hat{p} - i\hbar/2$, $\hat{g} = \hat{q}^2\hat{p}^2 - 2i\hbar\hat{q}\hat{p} + (i\hbar)^2/2 = \hat{f}^2 - \hbar^2/4$, so that $[\hat{f}, \hat{g}] = 0$, but $\hat{g} = \hat{W}(f^2) \neq \hat{f}^2$.

The failure of the squaring axiom is known as Temple's paradox (Temple 1935), and is the unpleasant property of *every* linear quantisation scheme. That is to say, the linearity of $\hat{W}: f \rightarrow \hat{f}$ is incompatible with the squaring axiom. There are arguments (Wan and McKenna 1982) that linearity should be dropped under certain conditions. From the practical point of view the failure of the squaring axiom implies severe difficulties in calculating the operators of the monomials of the normal form.

(C3) If f is a product of functions f_1 and f_2 , each of them depending on coordinates and momenta of different degrees of freedom, (i.e. f is factorially separated), then $[\hat{f}_1, \hat{f}_2] = 0$ and $\hat{f} = \hat{f}_1 \hat{f}_2$. Hence, in this special case the factorisation is satisfied: the image $\hat{W}(f_1 f_2)$ of a product of functions depending on different degrees of freedom is equal to the product of images, $\hat{W}(f_1 f_2) = \hat{W}(f_1) \hat{W}(f_2)$.

(C4) Among all linear quantisation rules the Weyl rule is distinguished by the covariance under the *linear* canonical transformations (Springborg 1983).

The property (C3) implies that the operator $\hat{W}(x^k y^l)$ corresponding to a monomial of (47) is decomposed into a product of operators corresponding to each degree of freedom,

$$\hat{W}(x^k y^l) = \hat{W}(x_1^{k_1} y_1^{l_1}) \dots \hat{W}(x_N^{k_N} y_N^{l_N}). \quad (48)$$

For one degree of freedom the Weyl rule is given by the formula (in usual notation)

$$\hat{W}(q^m p^n) = \frac{1}{2^n} \sum_{l=0}^n \binom{n}{l} \hat{p}^l \hat{q}^m \hat{p}^{n-l}, \quad (49)$$

or using the normal operator ordering (\hat{q} precedes \hat{p}),

$$\hat{W}(q^m p^n) = \sum_{l=0}^{\min(m,n)} \frac{(-i\hbar)^l l!}{2^l} \binom{m}{l} \binom{n}{l} \hat{q}^{m-l} \hat{p}^{n-l}. \quad (50)$$

In principle, equations (48)–(50) solve the correspondence problem $H \rightarrow \hat{H}$. The normal form for two degrees of freedom of order 8 has 495 monomials, and if each of them is mapped into a series of the form (50), containing about 100 terms, then this approach would be useless. It is thus necessary to find another representation, or to introduce approximations, or both, as we shall do.

The complex variables z_k and their conjugates z_k^* correspond precisely to the annihilation and creation operators, i.e.

$$\hat{z}_k = \hat{W}(z_k), \quad \hat{z}_k^+ = \hat{W}(z_k^*), \quad (51)$$

and their action on the eigenstates $|n_1, \dots, n_N\rangle$ of the harmonic operator \hat{H}_0 is

$$\begin{aligned} \hat{z}_k |n_1, \dots, n_k, \dots, n_N\rangle &= \sqrt{\hbar n_k} |n_1, \dots, n_k - 1, \dots, n_N\rangle, \\ \hat{z}_k^+ |n_1, \dots, n_k, \dots, n_N\rangle &= \sqrt{\hbar(n_k + 1)} |n_1, \dots, n_k + 1, \dots, n_N\rangle, \end{aligned} \quad (52)$$

where

$$\begin{aligned} k &= 1, 2, \dots, N, & n_k &= 0, 1, 2, \dots, \\ \hat{H}_0 |n_1, n_2, \dots, n_N\rangle &= \varepsilon_{n_1, \dots, n_N} |n_1, n_2, \dots, n_N\rangle, \\ \varepsilon_{n_1, n_2, \dots, n_N} &= \sum_{k=1}^N (n_k + \frac{1}{2}) \hbar \omega_k, \end{aligned} \quad (53)$$

with ε_n being the energy eigenvalues of \hat{H}_0 . The complex canonical variables (z, iz^*) thus seem to be more convenient than (x, y) . Indeed, from (27) we see that they are

canonically conjugate,

$$\{z_k, iz_l^*\} = \delta_{kl}. \tag{54}$$

Since they are related to (x, y) by the *linear* canonical transformation obtained from (18) upon multiplying by i , we can do the quantisation in this complex representation because of the property (C4).

We now show that the quantised normal form has the same fundamental property as the classical one, cf equations (5)–(6). Namely each monomial commutes with the harmonic part \hat{H}_0 of the Hamilton operator \hat{H} . Therefore the anharmonic part \hat{H}_A of the normal Hamiltonian, when quantised according to Weyl’s rule, commutes with \hat{H}_0 , and is thus diagonal in a harmonic basis. In § 6 we show that the integrability properties (5)–(6) are preserved under the quantisation.

Each monomial of the normal form, when represented in complex variables z, z^* , can be written as $z^m z^{*n}$, where $\omega(m - n) = 0$ (see (21)), which is equivalent to the vanishing of the Poisson bracket $\{H_0, z^m z^{*n}\}$. Now

$$H_0 = \sum_{j=1}^N \omega_j z_j z_j^* = \sum_{j=1}^N \omega_j \tau_j,$$

and thus by applying (50) one has

$$\hat{W}(\tau_j) = \hat{W}(z_j z_j^*) = \hat{z}_j^+ \hat{z}_j + \frac{1}{2}\hbar, \tag{55}$$

whence

$$\hat{H}_0 = \sum_{k=1}^N \omega_k (\hat{z}_k^+ \hat{z}_k + \frac{1}{2}\hbar). \tag{56}$$

By a straightforward calculation one can show that for one degree of freedom

$$[\hat{W}(z_k^{m_k} z_k^{*n_k}), \hat{W}(z_k z_k^*)] = i\hbar(m_k - n_k) \hat{W}(z_k^{m_k} z_k^{*n_k}).$$

By the property (C3) and the definition (55) we obtain the fundamental commutation relation of the quantised normal form, namely

$$[\hat{H}_0, \hat{W}(z^m z^n)] = i\hbar \omega(m - n) \hat{W}(z^m z^n). \tag{57}$$

This vanishes if and only if $\omega(m - n) = \sum_{k=1}^N \omega_k(m_k - n_k) = 0$, which is precisely the property of the monomials of the classical normal form. Hence, \hat{H}_A does indeed commute with \hat{H}_0 .

In this manner we can solve the quantisation problem $H \rightarrow \hat{H}$ by first expressing \hat{H} in terms of the complex variables, and then quantising it term by term according to Weyl’s rule. Taking into account the relation (51) we end up with \hat{H} expressed in terms of creation and annihilation operators $\hat{z}_k, \hat{z}_k^+, k = 1, \dots, N$.

The normal form expressed as a function of z, z^* is obtained from the general result (26) by inserting the definitions of τ_l and K_l . The operator corresponding to τ_l is given in (55). Let us calculate $\hat{W}(K_l)$. From the definitions (23)–(24) follows immediately

$$\hat{K}_l = \hat{u}_1^{|a_{l1}|} \dots \hat{u}_N^{|a_{lN}|}, \tag{58}$$

where

$$\hat{u}_k = \begin{cases} \hat{z}_k, & \text{if } a_{lk} \geq 0, \\ \hat{z}_k^+, & \text{if } a_{lk} < 0. \end{cases} \tag{59}$$

By $\hat{\tau} = (\hat{\tau}_1, \dots, \hat{\tau}_N)$ and $\hat{K} = (\hat{K}_1, \dots, \hat{K}_r)$ we denote the vectors of operators.

Because the squaring axiom is not satisfied (property (C2)), it is by no means sufficient to know the operators $\hat{\tau}$ and \hat{K} . The only consistent way of calculating \hat{H} cannot avoid the application of \hat{W} to each individual normal monomial $z^m z^{*n}$. But this results in an explosion of the expressions, which, after all, are not exact, because of the ambiguity in the fundamental problem of the quantisation scheme. Our goal is to obtain an algebraic quantisation algorithm which yields a good approximation for the spectrum, but is at the same time easy to handle. For this reason we now make a drastic approximation: we force the squaring axiom to hold. That is to say, we first calculate $\hat{\tau}$ and \hat{K} by using the Weyl rule, but then calculate \hat{H} by inserting them into the expression (26) as if the squaring axiom is satisfied. Note the important fact that the fundamental commutation relation $[\hat{H}_0, \hat{H}_A] = 0$ of the normal form is *not* destroyed by this approximation. Note also that this approximation is not necessary from the theoretical point of view, but is introduced to facilitate practical applications of the method. It is a reasonable assumption until a solution to the general quantisation problem has been found.

Let us now work out the implications of this approximation. First of all we can immediately write down the operator \hat{H} in terms of $\hat{\tau}$ and \hat{K} , cf (55) and (58)–(59),

$$\hat{H} = \sum_{\gamma} f_{\gamma}(\hat{\tau})(\hat{K}^{\gamma} + \hat{K}^{*\gamma}). \tag{60}$$

In non-resonant cases we have

$$\hat{H} = H(\hat{\tau}) = \sum_{k=1}^N \omega_k \hat{\tau}_k + H_A(\hat{\tau}_1, \dots, \hat{\tau}_N). \tag{61}$$

The energy spectrum is then simply given by

$$E_n = \sum_{k=1}^N \hbar \omega_k (n_k + \frac{1}{2}) + H_A((n_1 + \frac{1}{2})\hbar, \dots, (n_N + \frac{1}{2})\hbar), \tag{62}$$

where $n = (n_1, \dots, n_N)$ are non-negative integers (quantum numbers). The result is thus equivalent to the tori quantisation.

Example. For the fourth-degree normal form of example one in § 4 (see (42)), we get thus the energy spectrum

$$E_{n_1 n_2} = (n_1 + \frac{1}{2})\hbar \omega_1 + (n_2 + \frac{1}{2})\hbar \omega_2 + \hbar^2 \left[(n_1 + \frac{1}{2})(n_2 + \frac{1}{2}) \left(C + \frac{2\omega_2 c^2}{\omega_1^2 - 4\omega_2^2} \right) - (n_2 + \frac{1}{2})^2 \frac{c^2}{4\omega_1} \left(\frac{3\omega_1^2 - 8\omega_2^2}{\omega_1^2 - 4\omega_2^2} \right) \right], \quad n_1 n_2 = 0, 1, 2, \dots \tag{63}$$

Unlike in non-resonant cases, where \hat{H}_A is already diagonal in the harmonic basis, in resonant cases \hat{H}_A depends also on \hat{K} . Because \hat{K}_l is asymmetric product of \hat{z}_l and \hat{z}_l^* (different powers), \hat{H}_A is not *a priori* diagonal in the simple harmonic basis of \hat{H}_0 . Note that \hat{H}_0 has degenerate spectrum in the resonant case. An eigenspace of \hat{H}_0 has the dimension equal to the multiplicity ν of the eigenvalues $\varepsilon_{n_1, \dots, n_N}$. The eigenvalues A_{n_1, \dots, n_N} of \hat{H}_A are obtained if each block matrix $\langle n_1 \dots n_N | \hat{H}_A | n_1 \dots n_N \rangle$ corresponding to a (finite) eigenspace of \hat{H}_0 is diagonalised. Let us label the eigenvectors within an eigenspace by $m = 1, 2, \dots, \nu$. Then the eigenvalues A of \hat{H}_A are the solutions of the

secular equation

$$\det(A\delta_{mm'} - \langle m|\hat{H}_A|m'\rangle) = 0, \quad (64)$$

which completes the algebraic quantisation algorithm.

However, in the generic case that \hat{H}_A contains non-vanishing diagonal operators, i.e. if $f_{\gamma=(0,0,\dots,0)} \neq 0$ in (26), then we can use another, much more convenient, splitting of \hat{H} . Namely, we write \hat{H} as a sum of all diagonal operators summarised in \hat{H}_D and the non-diagonal (resonant terms) operators \hat{H}_R , i.e.

$$\hat{H} = \hat{H}_D + \hat{H}_R, \quad (65)$$

such that \hat{H}_D is diagonal on the harmonic basis $|n_1, \dots, n_N\rangle$, but no longer degenerate, as we included the anharmonic terms, while \hat{H}_R contains all terms depending on powers K^γ . In this event we are allowed to use the *non*-degenerate perturbation theory, taking \hat{H}_D as the unperturbed system and treating \hat{H}_R as a perturbation. We then have

$$E_n = D_n + \sum_{n' \neq n} |\langle n'|\hat{H}_R|n\rangle|^2 / (D_{n'} - D_n) + \dots \quad (66)$$

where $n := (n_1, n_2, \dots, n_N)$ and D_n denotes the eigenvalues of \hat{H}_D . The first-order term vanishes because the diagonal elements $\langle n|\tau^\alpha K^\beta|n\rangle$ vanish if the monomial $\tau^\alpha K^\beta$ is an asymmetric (in exponents) product of annihilation and creation operators. However, the formula (66) has a disadvantage that infinite matrices and their powers must be evaluated, while the procedure (64) involves only finite operations. We give now an example based on application of equation (64).

Example. Let us consider the six lowest energy levels of the normal form (fourth degree)

$$H = \tau_1 + \tau_2 + g_{20}\tau_1^2 + g_{11}\tau_1\tau_2 + g_{02}\tau_2^2 + \gamma_3(K^2 + K^{*2}). \quad (67)$$

Then, using the labelling $n = n_1 + n_2 + 1$, $m = 1, 2, \dots, \nu \leq n$

$$\begin{aligned} E_{11} &= \hbar + \frac{1}{4}\hbar^2(g_{20} + g_{11} + g_{02}), & E_{21} &= 2\hbar + \frac{1}{4}\hbar^2(9g_{20} + 3g_{11} + g_{02}), \\ E_{22} &= 2\hbar + \frac{1}{4}\hbar^2(g_{20} + 3g_{11} + 9g_{02}), \end{aligned} \quad (68)$$

$$E_{31} = 3\hbar + A_1, \quad E_{32} = 3\hbar + A_2, \quad E_{33} = 3\hbar + A_3,$$

where A_1, A_2, A_3 are the roots of the determinant

$$\det \begin{vmatrix} A - \frac{1}{4}\hbar^2(25g_{20} + 5g_{11} + g_{02}) & 0 & -2\gamma_3\hbar \\ 0 & A - \frac{9}{4}\hbar^2(g_{20} + g_{11} + g_{02}) & 0 \\ -2\gamma_3\hbar & 0 & A - \frac{1}{4}\hbar^2(g_{20} + 5g_{11} + 25g_{02}) \end{vmatrix} \quad (69)$$

whence

$$A_1 = \frac{9}{4}\hbar^2(g_{20} + g_{11} + g_{02}), \quad (70)$$

while A_2 and A_3 are the roots of a quadratic equation. Let us consider the numerical example (43) $\lambda = \frac{1}{10}$, $\eta = -\frac{1}{3}$, $\hbar = 1$ of the Hénon–Heiles system. We get

$$\begin{aligned} E_{11} &= 0.998\,7500, & E_{21} &= E_{22} = 1.992\,0833, \\ E_{31} &= E_{32} = 2.988\,7500, & E_{33} &= 2.965\,4167. \end{aligned} \quad (71)$$

This result is compared with the calculations by Weissman and Jortner (1982) in

table 3. The present method seems to be as accurate as perturbation theory, and much more accurate than the usual semiclassical quantisation.

Table 3. The lowest energy levels for the Hénon–Heiles system with $\lambda = \frac{1}{10}$, $\eta = -\frac{1}{3}$, $\hbar = 1$. We compare the results obtained by the present method (a) according to (67)–(71), with the results by Weissman and Jortner (1982): (b) ‘exact’ values, (c) quantum (second-order) perturbation theory, (d) the semiclassical quantisation.

	(a)	(b)	(c)	(d)
E_{11}	0.998 7500	0.998 88	0.998 89	0.995 83
E_{21}	1.992 0833	1.992 1	1.992 2	1.989 2
E_{33}	2.965 4167	2.965 1	2.965 6	2.962 5
E_{31}	2.988 7500	2.988 40	2.988 9	2.985 8

In an erratum Swimm and Delos confirm that the results given in their table II (1979) do indeed refer to $\lambda = 1/\sqrt{80}$, (not $\lambda = 1/80$) so that we are able to compare their results with predictions of the present method. Table 4 clearly shows the excellent accuracy of the present method: note that we have quantised the fourth-degree normal form while Swimm and Delos took eighth degree, and yet our results are much more accurate.

Table 4. The lowest energy levels for the Hénon–Heiles system with $\lambda = 1/\sqrt{80}$, $\eta = -\frac{1}{3}$, $\hbar = 1$. We compare the results obtained by the present method (fourth-degree normal form) (a) with the ‘exact’ quantum mechanical calculations by Noid as listed in Swimm and Delos (b), the tori quantisation results (eighth-degree normal form) by Swimm and Delos (1979) (c), and the semiclassical results by Noid and Marcus (1977) (d).

	(a)	(b)	(c)	(d)
E_{11}	0.998 4375	0.9986	0.9947	0.9947
E_{21}	1.990 1042	1.9901	1.9862	1.9863
E_{33}	2.956 7708	2.9562	2.9506	2.9506
E_{31}	2.985 9375	2.9853	2.9814	2.9815

We summarise, and stress the major steps of the quantisation method when applied to specific examples.

(i) For the given (classical) Hamiltonian (10) one has to calculate the normal form (26) to the desired order, using the algorithm of §§ 1 and 2.

(ii) The basic variables $\tau = (\tau_1, \dots, \tau_N)$ and $K = (K_1, \dots, K_r)$ are then replaced by their Weyl correspondents $\hat{\tau}$ and \hat{K} , which are further expressed in terms of the ladder operators according to (55) and (59).

(iii) In the non-resonant case the energy spectrum is obtained simply by replacing τ_k by $(n_k + \frac{1}{2})\hbar$, where $n_k = 0, 1, 2, \dots$ are the quantum numbers, $1 \leq k \leq N$. So, no operators are needed here to calculate the energy levels.

(iv) In the resonant case one has to diagonalise the anharmonic part \hat{H}_A of the normal Hamiltonian in the finite subspaces of the harmonic operator. Thus by solving the eigenvalue problem (64) for each of the finite subspaces we find a basis so that \hat{H}_A is diagonal and the degeneracy of \hat{H}_0 on the subspace is removed.

6. Problems related to the quantum integrability

Let a quantum mechanical system be determined by the Hamilton operator

$$\hat{H} = \hat{H}(\hat{q}, \hat{p}), \quad (72)$$

where $\hat{q} = (\hat{q}_1, \dots, \hat{q}_N)$, $\hat{p} = (\hat{p}_1, \dots, \hat{p}_N)$ obey the canonical commutation relations

$$[\hat{q}_k, \hat{q}_l] = [\hat{p}_k, \hat{p}_l] = 0, \quad [\hat{q}_k, \hat{p}_l] = i\hbar \delta_{kl}. \quad (73)$$

We define \hat{H} to be integrable if there are N (= number of degrees of freedom) independent, mutually commuting observables

$$\hat{F}_i = \hat{F}_i(\hat{q}, \hat{p}), \quad 1 \leq i \leq N, \quad [\hat{F}_i, \hat{F}_j] = 0, \quad (74)$$

one of them, say \hat{F}_1 , being the Hamilton operator itself, and each of them being a function of the operators \hat{q} and \hat{p} . (We thus exclude observables related to discrete symmetries.)

Defined in this way, the integrability is a purely quantum mechanical property and can be in principle investigated by the theories on algebras of operators in the Hilbert spaces, without reference to classical mechanics. However, little is known on the general integrability properties of quantum systems. The question is important, as it is related to the existence of the (exact) quantum numbers: if a system is integrable, then it has N quantum numbers. If it is not integrable, then the question arises, how many exact quantum numbers exist.

The problem in its whole generality cannot be solved unless the basic problem of the quantisation prescription is solved. The solution of the latter will at the same time enable us to study also the correspondence between the classical and quantum integrability. In view of the enormous difficulties that we face the following question is of heuristic importance: what does the classical integrability imply for the corresponding quantum system? The classical integrability is somehow better understood, albeit no general decision or construction algorithm for integrable systems is known to date (see Holt 1982). One should not forget that the results and conclusions of such investigations are dependent on (and probably sensitive to) the choice of the correspondence rule $\hat{W}: f \rightarrow \hat{f}$.

With this in mind I present now some partial results on the quantum integrability. Let (26) be the normal form of a classical Hamilton system (10). The infinite formal series of the normal form can *accidentally* terminate. (The exact condition for termination is not known, but it can be seen from the strong coupling of terms through equation (16) that this is a rare event. If each term $H^{(j)}$, $j > 2r$, should vanish, then this imposes conditions on all terms for which $r < j < 2r$.) If this happens then the Hamilton system (10) is integrable. We now show that if (A) the operators of the normal variables (x, y) satisfy the commutation relations (45), and if (B) $\hat{W}: f \rightarrow \hat{f}$ is the Weyl correspondence rule, then the corresponding normal Hamiltonian has quantum integrals which are precisely the Weyl correspondents of the classical integrals (7) and (8), for the non-resonant and resonant case, respectively.

To show this we use the complex representation, which is permitted by the property (C4). Then the classical normal Hamiltonian reads

$$H = H_0 + H_A = \sum_{k=1}^N \omega_k z_k z_k^* + \sum_{m,n} h_{mn} (\text{mon}) z^m z^{*n}. \quad (75)$$

In the non-resonant case $m = n$, $(zz^*)^m = \tau_1^{m_1} \dots \tau_N^{m_N}$, and it is thus sufficient to show that

$$[\hat{W}_{ii}, \hat{W}_{jj}] = 0 \tag{76}$$

for any $i, j = 0, 1, 2, \dots$, where

$$\hat{W}_{kl} = \hat{W}(q^k p^l)$$

is the Weyl correspondent of the (one-dimensional) monomial $q^k p^l$. But (76) can be verified by applying the formula (50). The operators $\hat{\tau}_k = \hat{W}(z_k z_k^*)$ thus commute with each $\hat{W}(z_k^i z_k^{*j}) = \hat{W}(\tau_k^i)$, and therefore with $\hat{H} = \hat{W}(H)$.

In the resonant case we have to show that for each $1 \leq l \leq N - r$,

$$\hat{I}_l = \sum_{k=1}^N \mu_{lk} \hat{\tau}_k \tag{77}$$

commutes with \hat{H} . But this follows immediately, *mutatis mutandis*, from (57): instead of the factor $\omega(m - n)$ or the RHS of (57) we obtain

$$\sum_{k=1}^N \mu_{lk} (m_k - n_k). \tag{78}$$

Since $m_k - n_k$ is a linear combination of the rows of the matrix a_{lk} (cf (4) and (22)), the factor (78) is zero. Therefore (77) are the quantum integrals of the motion, since they commute with \hat{H} and among themselves.

7. The relation to quantum mechanical perturbation theory: an example

Consider the Hamilton system

$$H = \frac{1}{2}\omega_1(x_1^2 + y_1^2) + \frac{1}{2}\omega_2(x_2^2 + y_2^2) + cx_1x_2^2 + Cx_1^2x_2^2. \tag{79}$$

Its normal form has been given in (42) and the resulting energy levels in (63). Let us now compare this result with the purely quantum mechanical perturbation theory as applied to the original system (79). Then we have (up to the second order in \hbar)

$$E_{n_1, n_2} = \varepsilon_{n_1, n_2} + \langle n_1, n_2 | Cx_1^2x_2^2 | n_1, n_2 \rangle + \sum_{(n'_1, n'_2) \neq (n_1, n_2)} \frac{|\langle n_1, n_2 | Cx_1x_2^2 | n'_1, n'_2 \rangle|^2}{\varepsilon_{n_1, n_2} - \varepsilon_{n'_1, n'_2}}. \tag{80}$$

The calculation of (80) is straightforward and the result is surprisingly close to the spectrum (79) of the normal form. Namely, (to the second order in \hbar) they differ only by an additive *constant* of order \hbar^2 , i.e.

$$E_{n_1, n_2}(\text{Birkhoff-Gustavson}) - E_{n_1, n_2}(\text{perturbation theory}) = \frac{3}{16}c^2\hbar^2 \omega_1/(\omega_1^2 - 4\omega_2^2). \tag{81}$$

The question is now which approximation is closer to the (unknown) exact result. Such a comparison is possible in one-dimensional cases, $N = 1$. Clearly, Birkhoff-Gustavson normal form for these integrable systems is just an algebraic method of the power expansion of the Hamiltonian in terms of the action variable. A similar result has been obtained for them: (to the second order) the spectra differ only by an additive constant. If the results are then compared with exactly soluble systems it is found that in the case of the Morse potential the additive constant incidentally vanishes

and both results are exact. However, in the case of the potential $U(x) = a/x + b/x^2$ we find that the Birkhoff–Gustavson spectrum is closer to the exact result than the perturbation theory.

8. The transition probabilities

The important achievement of the present quantisation method is that we are able to calculate the matrix elements and therefore the transition probabilities for electromagnetic transitions. This is an advantage of the method as compared with a purely semiclassical tori quantisation (cf Swimm and Delos 1979).

We remind the reader that by the quantisation procedure of § 5 we get simultaneously also the eigenstates, which are finite linear combinations of the simple harmonic functions. For example, to calculate the dipole transitions, we have then to know the matrix elements

$$W_{if} = \langle \Psi_i | \mathbf{r} | \Psi_f \rangle, \quad (82)$$

where the initial and the final states Ψ_i and Ψ_f are finite linear combinations of states $|n_1, \dots, n_N\rangle$. To calculate (82) one has to express the dipole term \mathbf{r} as a function of the normal coordinates and momenta (by inverting the canonical transformations), $\mathbf{r} = \mathbf{r}(x, y)$, and then to express x, y in terms of the annihilation and creation operators.

9. Discussion and conclusion

In this work we have reviewed the algorithm leading to the Birkhoff–Gustavson normal form for Hamiltonians that can be power expanded around an equilibrium point. We have found the most general expression for the normal form and derived some of its properties. The algebraic quantisation has been achieved by means of the Weyl quantisation rule, and the normal form Hamiltonian has been expressed in terms of the annihilation and creation operators. This allows us to calculate the energy levels, and the transition probabilities. We gave several analytic examples, including the most general solution for the fourth-degree normal form for two degrees of freedom (the resonance $\omega_1/\omega_2 = \frac{1}{2}$ being excluded). We further compared the results with numerical works by Gustavson (1966), Swimm and Delos (1979) and Weissman and Jortner (1982). Finally, by means of an example, we compared the energy levels obtained by the present method with the predictions of the (second-order non-degenerate) perturbation theory, where a surprisingly good agreement has been found.

It remains to comment on the non-integrability and stochasticity. As pointed out in the introduction, the absence of classical integrals of motion is related to the divergence of the perturbation series. The consequence is the instability of trajectories and the onset of chaotic behaviour, which fully develops at the critical energy (stochastic transition). At energies above the critical energy the formal integrals of motion have no meaning, while below the stochastic transition they provide a good analytical approximation for the invariant tori.

The consequences of non-integrability in quantum mechanics are not so clear and are still discussed (Berry 1982, 1983, Zaslavsky 1981, Robnik 1981, 1982a, b). We consider here the stationary problem. For the classical integrable Hamiltonian systems

we have the well known tori quantisation, initiated by Einstein and further developed by Maslov. In non-integrable cases one uses the Feynman path integrals to evaluate the *semiclassical* propagator in order to calculate the level density. This turns out to be given by a sum over closed classical orbits (Gutzwiller 1978, Berry 1983, Zaslavsky 1979, Berry and Tabor 1976, 1977).

One of the most important consequences of a stochastic transition (integrable \rightarrow non-integrable) is a drastic change of the probability density $P(S)$ for the spacings S between two adjacent energy levels. In integrable systems, where level crossings are allowed, we have a distribution of uncorrelated objects and $P(S) = \exp(-S)$ is a Poisson distribution, showing that $P(S) \rightarrow \text{constant} \neq 0$ as $S \rightarrow 0$. For sufficiently chaotic systems (say, K -systems) the levels repel each other, their crossings are forbidden, implying a strong correlation. As a result of this $P(S)$ is a Wigner-type distribution, i.e. $P(S) \propto \exp(-S^2)$ for $S \gg 1$ and obeys a power law $P(S) \rightarrow S^\nu$ as $S \rightarrow 0$, reflecting the fact that level crossings are not allowed. The goal of the theory is to predict the critical exponent ν by deriving it from the dynamical properties of the system rather than by using some randomness hypothesis for the matrix elements of the Hamiltonian.

Such a stochastic transition in the distribution of level spacings has been known observationally in nuclear and atomic physics for quite a long time (see e.g. Rosenzweig and Porter 1960). The stochastic transition in an interesting class of plane billiards with analytic boundaries has been investigated recently (Robnik 1983). It is somehow urgent to further develop the theory.

There is another property of the energy levels related to the classically integrable or chaotic motion, which has been predicted by Percival (1973) and observed by Pomphrey (1974): levels corresponding to the regions of the phase space with integrable motion are stable with respect to the parameters of the Hamiltonian, while levels corresponding to the chaotic classical motion are unstable. They are called regular and irregular levels, respectively. A purely quantum mechanical stability theory of the spectra of Schrödinger operators (Vock and Hunziker 1982) now in progress might provide a rigorous confirmation of Percival's semiclassical prediction (cf Robnik and Zaslavsky 1983). It should be noted at this stage, however, that according to the recent calculations by Weissman and Jortner (1982) there is no evidence for the irregular, unstable levels for the Hénon–Heiles system, in contrast to the observations by Pomphrey (1974), where the spectrum is ‘condensed’ due to the ten times smaller value of the coupling parameter λ . Therefore Pomphrey's system is closer to the classical limit, as has been pointed out by Noid *et al* (1980).

There is a connection between the two properties, the common origin of both being the crossings or repulsions of levels. Namely, as a result of level repulsions the energy levels as a function of some parameter of the Hamiltonian do *not* change smoothly as would be the case for an integrable system. The instability of levels and the stochastic transition of the distribution $P(S)$ must be therefore related to the divergence of the quantum mechanical perturbation series: if the series were convergent, then the energy levels would be smooth (in fact analytic) functions of the parameters. Consequently, the energy levels as predicted by the quantisation of the Birkhoff–Gustavson normal form can be accurate as long as the exact levels are stable, regular. In regions of irregular levels the quantisation of the normal form can hardly predict the fine structure of the spectrum, but it very likely does predict the mean level density correctly. To derive the distribution $P(S)$ there one cannot avoid solving the basic problem of predicting $P(S)$ by the true dynamical properties of the Hamiltonian, or calculating $P(S)$ by using the exact energy levels.

Acknowledgments

I wish to thank Dr Eberhard Schrüfer (University of Bonn) for valuable comments and many stimulating discussions. Helpful comments by R A Marcus are gratefully acknowledged. Finally, sincere thanks are due to George M Zaslavsky for stimulating discussions through the letters we exchanged over the past year. This work was not supported by any military agency.

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