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The proper quantum analogue of the Birkhoff–Gustavson method of normal forms

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Abstract. A deformation approach resolves problems concerning the ordering of operators and the commutation of quantization with canonical transformation. This completes the programme of Robnik to develop a purely algebraic method for the quantization of non-integrable Hamiltonian systems about a point of stable equilibrium.

1. Introduction

The aim of this work is to provide a quantum analogue for the method of normal forms. Almost all Hamiltonian systems are non-integrable. It is a general feature of non-integrable systems, however, that at energies in the neighbourhood of a stable equilibrium, they possess many of the properties which characterize integrable ones. They behave regularly, and trajectories are confined to lie on ‘invariant tori’, n -dimensional surfaces in the $2n$ -dimensional phase space. The presence of such tori suggests the existence of approximate integrals of the motion. As the energy of a system is increased, the surfaces confining the trajectories distort. Associated with this distortion are period-doubling phenomena and bifurcations in the Poincaré surfaces of section. The distorted tori eventually break up into ‘cantori’, complicated structures like Cantor sets, where the trajectories are divided into islands, or families of trajectories, alternately describing chaotic and regular motion. As the energy is further increased the space occupied by the irregular trajectories grows in volume until at a certain critical energy all motions become chaotic. The trajectories are no longer confined to n -dimensional tori but wander to fill the whole energy surface. This is one of the well known routes to chaos [1] and has been extensively studied numerically. The method of normal forms was developed by Birkhoff to predict the presence of invariant tori (approximate integrals of the motion), the bifurcation of tori and the general behaviour of classical systems in the sub-critical energy regime.

The Hamiltonian is expanded as a Taylor series about the point of stable equilibrium. The lowest-order terms resemble a series of uncoupled harmonic oscillators. The idea is to transform the Hamiltonian by a series of canonical transformations, so that to progressively higher orders, H commutes with the harmonic terms in the lowest order. The harmonic part, that which commutes with the lowest-order component of H , constitutes an integrable, low-energy effective model for the original system. By including higher-order harmonic components we get a system which is still integrable,

is somehow close to the original non-integrable system and (it is expected) models the behaviour of the original system as long as the islands of regular motion persist.

It became apparent that the method of normal forms would provide a quick and easy approach to the quantization of non-integrable or non-separable systems. The value of such an approach is not so much in calculating spectra (there are other methods), but in providing an effective integrable model which accurately reproduces the features of the non-integrable system in the sub-critical energy regime, and which enables one to understand the quantum mechanics of a classically chaotic system in terms of approximate quantum numbers and approximate conservation laws. This method has had applications in the study of the vibrational energy flow in molecules [2-4], laser-induced multiphoton photodissociation in molecules [5], and in the study of the quadratic Zeeman effect for the hydrogen atom in a strong magnetic field [6,7].

The method of normal forms has also had a role to play in the search for, and investigation of quantum chaos. Indeed this has been one of the big industries of modern physics; for a recent review of current problems see Elyutin [8]. One approach in the search for a characterization of quantum chaos is based on the behaviour of the invariant tori breaking up to signal the onset of chaos. The method of normal forms is essentially a torus quantization, the naive expectation was therefore that the method should be accurate as long as these tori persist, breaking down thereafter [9]. This approach was adopted by Swimm and Delos [10] to carry out the quantization of certain non-integrable Hamiltonian systems about a point of stable equilibrium. Very good results were obtained in many cases giving better results than ordinary perturbation theory [10]. However the expected failure of the method does not seem to occur. Calculations for the Hénon-Heiles system revealed that the method gives good results well into the chaotic regime, and even beyond the dissociation energy [10, 11]. In the resonant case, their method involved numerically computing the actions $\oint p dq$, obtained by integrating around various orbits in phase space. Robnik improved on this situation by developing a fully algebraic method of quantization [9]. This cut out the need for numerical integrations and moved away from the use of torus quantization. His method however relied on a number of working assumptions. It was assumed:

(1) that the polynomials arising in the classical expression for the normal form represent Weyl-ordered operators;

(2) that the transformed quantum canonical coordinates q' and p' , satisfy the same fundamental bracket relations as their predecessors q, p ; and

(3) that a generalization of the squaring axiom holds. For example if ω_W is Weyl-ordering, then it is taken (wrongly of course [9, 12]) that the following is true:

$$\omega_W \circ (q^2 + p^2)^n = [\omega_W \circ (q^2 + p^2)]^n.$$

The central issues here are the commutation of quantization with canonical transformation (CT), and the need for an efficient formalism to deal with the ordering of complicated polynomial expressions in the Heisenberg-Weyl algebra. Most classical CTs are local and they do not extend to global changes of variables. For instance the transformation from Cartesian to polar coordinates is not one-to-one invertible, but changes the topology of the configuration space. This raises issues relating to the existence and uniqueness of representations of the Heisenberg-Weyl algebra. The only classical CTs which do commute with quantization are those which are continuously connected to the identity. These are infinitesimally generated, and their quantum analogues are the unitary transformations—obtained by the complex exponentiation of self-adjoint operators.

Independent work by Eckhardt [13], and by Ali [14], demonstrates that in the classical method of normal forms, the construction of canonical transformations using generating functions, can be replaced by an approach using Lie transforms. Within this framework they replace the Lie brackets, with the commutators of the quantum algebra, to produce a quantum method of normal forms very similar to our own. They point out that this is probably equivalent to Rayleigh-Schrödinger perturbation theory, and Ali gives an argument as to why this should be so. However the questions concerning the ordering of operators, and a method of normal forms which commutes with the quantization process remain unsolved. The problem of understanding the relationship between classical and quantum integrable systems has been looked at by Hietarinta [15].

We resolve the problems concerning the commutation of quantization and CT on \mathbb{R}^d by quantizing in the frame in which the system is understood, and by working thereafter in terms of quantum CTs. We resolve the problem of handling complicated expressions in the Heisenberg-Weyl ring by using the formalism which we present in the next section.

2. Tools and terminology

The quantization of a classical Hamiltonian system can be thought of as the process by which the classical algebra of observables is replaced with the quantum algebra of observables. The Poisson bracket acting on functions of phase space is replaced with the commutator algebra of operators acting on functions of configuration space. Quantization can be studied as a deformation of the classical algebra of observables. For an introduction to the philosophy of the deformation approach and an overview of its possible scope see Flato [16]. The theory of the deformations of Lie algebras has drawn from the work of Moyal [17], Agarwaal and Wolf [18], Vey [19], Lichnerowicz [20], Gerstenhaber [21], Bayen *et al* [22], and more recently by Dunne [23]. This approach provides an insightful reformulation of quantum mechanics in which the Heisenberg-Weyl algebra is recognized to be the unique non-trivial deformation of the classical algebra of observables on \mathbb{R}^d , in which the observables are those of classical mechanics, and the energy is quantized as in quantum theory. An adaptation of the formalism summarized by Niederle [24] provides an ideal tool with which to develop the quantum analogue of the method of normal forms.

In associating a quantum observable with some classical observable, ordering problems may arise [25]. When they do the only distinguished choice of ordering is Weyl-ordering. This is distinguished by the fact that it commutes quantization with linear CTs. Otherwise we are free to associate with a classical observable, any quantum operator with the same dimension and a non-singular limit as $\hbar \rightarrow 0$.

Let $O(q, p)$ be the space of classical polynomial observables. $O_{\hbar}(q, p, \hbar)$ is the space of extended classical polynomial observables. In this case the algebra is classical, but the functions are allowed a formal dependence on \hbar . \overline{W} is the Heisenberg-Weyl ring, the space of quantum polynomial observables in which the q, p, \hbar obey the following fundamental bracket relations:

$$[q_i, q_j] = 0$$

$$[q_i, p_j] = i\hbar\delta_{ij}$$

$$[p_i, p_j] = 0.$$

Quantization is a mapping from $O_{\hbar}(q, p, \hbar)$ to \overline{W} . This is not an algebraic isomorphism, it is a re-interpretation of the symbols in $O_{\hbar}(q, p, \hbar)$ as Weyl-ordered operators. Since every polynomial operator can be expressed as a sum of Weyl-ordered operators, the ordering problem is that of choosing an embedding of $O(q, p)$ in $O_{\hbar}(q, p, \hbar)$, and quantization is the natural association of each symbol in $O_{\hbar}(q, p, \hbar)$ with a Weyl-ordered operator in \overline{W} . It is convenient to represent the elements of \overline{W} by their symbols in $O_{\hbar}(q, p, \hbar)$ instead of complicated expressions involving orderings of operators.

\overline{W}^s is the envelope of all monomials $q^i p^j \hbar^k$ where $|i| + |j| + 2k = s$, and $i, j, k \geq 0$. The i, j are vectors of dimension d , the dimension of configuration space. $|i|$ stands for $i_1 + \dots + i_d$. This provides a partition of the Heisenberg-Weyl ring \overline{W} , as follows

$$\overline{W} = \overline{W}^0 \oplus \overline{W}^1 \oplus \overline{W}^2 \oplus \dots$$

The monomials $q^i p^j \hbar^k$ are the quantum analogues of monomials which figure in the classical method of normal forms, $q^i p^j$ where $i + j = s$ [10, 26].

It is generally appreciated that the product of two Weyl symbols is not the Weyl symbol of the product, but the Weyl symbol of the Moyal product [17]. The Moyal product of two operators f, g is denoted $f * g$, and maps $\overline{W} \times \overline{W} \rightarrow \overline{W}$, and is given by

$$f * g = \exp \left(i \frac{\hbar}{2} (\partial_{q_1} \partial_{p_2} - \partial_{p_1} \partial_{q_2}) \right) f(q_1, p_1) g(q_2, p_2). \quad (1)$$

It is assumed that, having calculated such an expression (1), the substitutions $q_1 = q_2 = q$, and $p_1 = p_2 = p$ are made. Similarly the Weyl symbol for the commutator of two Weyl symbols is not the Poisson bracket, but the Moyal bracket of the symbols [17]:

$$[f, g] = f * g - g * f = 2i \sin \left(\frac{\hbar}{2} (\partial_{q_1} \partial_{p_2} - \partial_{p_1} \partial_{q_2}) \right). \quad (2)$$

We can work exclusively in terms of the Weyl symbols without the need to re-order our expressions at various stages in each calculation. We will find it desirable to express Weyl-ordered symbols in terms of objects representing operators in some other ordering, for example standard-ordering. Given a symbol W , representing an operator in some ordering i , the symbol which represents the same operator but in a different ordering j , can be calculated from the original one by applying a deformation σ_i^j to W . There is no confusion as long as one remembers which ordering the symbols represent. The set of all σ_i^j form a group and we will have occasion to use these in section 4.2. With this machinery at our disposal we are now ready to look at the method.

3. The method

A Hamiltonian system is represented by the Taylor expansion of the Hamiltonian function about a point of stable equilibrium. In this form $H = \sum_{s=2} H^s$, where $H^s \in \overline{W}^s$, and $H^2 = \sum_{k=2} \omega_k T_k$. The T_k are harmonic oscillator terms $(p_k^2 + q_k^2)/2$. We say that H is harmonic to order n , if $H^k \in K(H^2) \forall k \leq n$, where $K(H^2)$ is

defined by the property $[X, H^2] = 0$ for all $X \in K(H^2)$. Hamiltonians in which the lowest-order terms are harmonic oscillators, and in which higher terms are harmonic to order n , are said to be in 'normal form' to that order [26].

We will now describe a way for generating transformations of the Hamiltonian H , so that the new Hamiltonian H' is in normal form to successively higher orders. We assume that $H^{i'} \in K(H^2)$ for $i = 1, \dots, s-1$ and look for a unitary transformation which transforms H into H' , so that $H^{i'} \in K(H^2)$ for $i = 1, \dots, s$. Take $W^s \in \overline{W}^s$, and H' as follows

$$\begin{aligned} H' &= \exp(iW^s/\hbar)H\exp(-iW^s/\hbar) \\ &= H + [W^s, H] \left(\frac{i}{\hbar}\right) + \frac{1}{2!}[W^s, [W^s, H]] \left(\frac{i}{\hbar}\right)^2 + \dots \end{aligned}$$

The transformed Hamiltonian can be written in the form

$$H' = H'^2 + H'^3 + \dots + H'^s + \dots \quad H'^t \in \overline{W}^t \quad \forall t.$$

Notice that if $W^s \in \overline{W}^s$ and $H^i \in \overline{W}^i$, then

$$\overbrace{[W^s, [W^s, \dots [W^s, H^i] \dots]]}^{n\text{-times}} \left(\frac{i}{\hbar}\right)^n \in \overline{W}^{n(s-2)+i} \quad \forall i, s, n.$$

On inspection we find that $H^{i'} = H^i$ for $i = 2, \dots, s-1$. That is H is unaltered to order $s-1$. The term of order s is given by

$$H'^s = H^s + [W^s, H^2] \left(\frac{i}{\hbar}\right) \quad (3)$$

and the general term, by the following formula

$$H'^n = \sum_{j(s-2)+k=n} \overbrace{[W^s, \dots, [W^s, H^k] \dots]}^{j\text{-times}} \left(\frac{i}{\hbar}\right)^j \frac{1}{j!}. \quad (4)$$

Choosing W^s so that $H'^s \in K(H^2)$, we ensure that H' is in normal form to order s . The existence of a solution is guaranteed by construction; however it is far from being unique. Given one solution W^s any element of $W^s \oplus (K(H^2) \cap \overline{W}^s)$ is also a solution. The simplest and most convenient choice is $W^s \in K(H^2)^c$.

Before we can construct the solution, we need to elucidate the structure of $K(H^2)$. Assume that $\Phi \in K(H^2)$. From (2) we have that

$$\begin{aligned} [H^2(q, p), \Phi(q, p)] &= 2i \sin \left(\frac{\hbar}{2} (\partial_{q_1} \cdot \partial_{p_2} - \partial_{q_2} \cdot \partial_{p_1}) \right) H^2(q_1, p_1) \Phi(q_2, p_2) \\ &= 2i \sum_k \omega_k \left(p_k \frac{\partial \Phi}{\partial q_k} - q_k \frac{\partial \Phi}{\partial p_k} \right) \\ &= 0. \end{aligned}$$

Therefore Φ must satisfy $\sum_k \omega_k (p_k \partial_{q_k} - q_k \partial_{p_k}) \Phi = 0$. To find all solutions of this we go to the coordinate representation defined by

$$p_k = \frac{1}{\sqrt{2}}(e_k + i n_k) \quad q_k = \frac{i}{\sqrt{2}}(e_k - i n_k).$$

In this representation, $\phi \in K(H^2)$ if and only if $\sum_k \omega_k (e_k \partial_{e_k} - n_k \partial_{n_k}) \Phi = 0$. Taking $\Phi = e^l n^m$ (shorthand for $e_1^{l_1} \cdots e_n^{l_n} n_1^{m_1} \cdots n_n^{m_n}$), this becomes, $\sum_k \omega_k (l_k - m_k) \Phi = 0$, and $\phi = e^l n^m$ lies in $K(H^2)$ if and only if

$$\sum_k \omega_k (l_k - m_k) = 0. \quad (5)$$

To complete the calculation, W^s and H^s are expressed in the form

$$H^s = \sum_{|l|+|m|+2k=s} e^l n^m \hbar^k \alpha_{lmk} \quad W^s = \sum_{|l|+|m|+2k=s} e^l n^m \hbar^k \beta_{lmk}.$$

Equation (3) for H'^s becomes

$$H'^s = \sum_{|l|+|m|+2k=s} e^l n^m \hbar^k [\alpha_{lmk} + \omega \cdot (l - m) \beta_{lmk}]. \quad (6)$$

The coefficients α_{lmk} are known, but the β_{lmk} are determined so that $H'^s \in K(H^2)$. This is achieved by choosing β_{lmk} as follows

$$\beta_{lmk} = \alpha_{lmk} / \omega \cdot (l - m) \quad \text{when} \quad \omega \cdot (l - m) \neq 0. \quad (7)$$

It does not matter what we choose when $\omega \cdot (l - m) = 0$. The choice $W^s \in K(H^2)^c$, given by

$$\beta_{lmk} = 0 \quad \text{when} \quad \omega \cdot (l - m) = 0 \quad (8)$$

is optimal in that it cuts down on calculations by having as many terms as possible equal to zero. From (7) and (8), W^s can be found, and the new Hamiltonian calculated. H' is in normal form to degree s , and the whole procedure can be repeated to transform H to normal form to as high a degree as required.

The polynomials W^i are Hermitian operators. The complex exponentiation of an Hermitian operator gives an isometry which is Hermitian. The W^i always have self-adjoint extensions [27] which provide unitary transformations of the Hilbert space. The difference between different extensions is not manifest in the spectrum of the truncated normal form. This is not where the story ends however. Each term arising in the resulting normal form represents a Weyl-ordered partial differential operator, we must now address.

4. The spectral problem

Hamiltonians about points of stable local equilibrium fall into one of two categories. They are distinguished by whether or not ω_k , the fundamental frequencies, satisfy the following condition of commensurability:

$$\forall k \exists a_k \in \mathcal{Z} \text{ such that some } a_k \neq 0 \quad \text{and} \quad \sum_{k=0}^d a_k \omega_k = 0. \quad (9)$$

Those which do are referred to as 'resonant' Hamiltonians, and those which do not are referred to as 'non-resonant'. Geometrically, an orbit of an integrable non-resonant Hamiltonian systems fills out the n -dimensional invariant torus on which it lies. In the resonant case, however, a single orbit is confined to a lower dimensional subset of this torus. From an algebraic point of view, the only monomials $e^{l_1} \dots e^{l_d} n^{m_1} \dots n^{m_d}$ which lie in $K(H^2)$ occur for $l_k = m_k \forall k$. In this case $K(H^2)$ is composed of arbitrary functions of T_1, \dots, T_d , the harmonic oscillators. In particular if H is in normal form to order t then H_h , the normal part of H is given by

$$H_h = \sum_{k=2}^t H^k(T_1, \dots, T_d). \quad (10)$$

The eigenfunctions of the T_k are given by ψ_k^n and satisfy:

$$T_k \psi_k^n = \hbar(n_k + \frac{1}{2}) \psi_k^n \quad n_k = 0, 1, 2, \dots \quad (11)$$

Birkhoff and Gustavson [26], made the assumption that given $\psi_k^{n_k}, T_k$ satisfying (11), the wavefunctions of H^h are provided by

$$\Psi_{n_1 \dots n_d} = \psi_1^{n_1} \dots \psi_d^{n_d} \quad (12)$$

where $n_1, \dots, n_d \in \mathcal{Z}^+$, and that the spectral problem is resolved as follows

$$H^h(T_1, \dots, T_d) \Psi_{n_1 \dots n_d} = H^h[\hbar(n_1 + \frac{1}{2}), \dots, \hbar(n_d + \frac{1}{2})] \Psi_{n_1 \dots n_d}. \quad (13)$$

However this is not true. This was a valid working assumption in the context of the semi classical method because it was not known how to order the complicated expressions which arose. We now look at how to overcome the problem presented by the failure of (13) to hold.

4.1. Non-resonant Hamiltonians

Since each group of variables q_i, p_i , or equivalently e_i, n_i , commutes with each other group, we need only consider the problem of the spectrum of T_k^t for arbitrary k . We therefore drop the subscript and start by looking at what happens to T^t .

While it is not true that

$$T^k \psi^n = [\hbar(n + \frac{1}{2})]^k \psi^n$$

it is true that

$$(*T)^k \psi^n = [\hbar(n + \frac{1}{2})]^k \psi^n.$$

The notation $(*T)^k$ is shorthand for the Moyal product of T k -times. We need to express T^k in terms of the products $(*T)^k$. Repeatedly applying the rule for the Moyal product of two factors $A_2 * A_1$ (1), we get the rule for the Moyal product of m factors. This is given by the following deformation of the corresponding classical product.

$$A_m * \cdots * A_1 = \exp \left(i \frac{\hbar}{2} \sum_{i,j} \Delta_m^{ij} \partial n_i \cdot \partial e_j \right) A_m(e_m, n_m) \cdots A_1(e_1, n_1) \quad (14)$$

where $i, j \in \{1, \dots, m\}$ and

$$\begin{aligned} \Delta_m^{ij} &= +1 & i > j \\ &= 0 & i = j \\ &= -1 & i < j. \end{aligned}$$

It is assumed that after evaluation of the expression we set each $e_i = e$, and each $n_i = n$. Taking $d = 1$ and setting each $A_i(e, n) = e_i n_i \forall i = 1, \dots, m$, the identity (14) becomes

$$\begin{aligned} (*en)^m &= \exp \left(i \frac{\hbar}{2} \sum_{i,j} \Delta_m^{ij} \partial n_i \partial e_j \right) (e_m n_m) \cdots (e_1 n_1) \\ &= \prod_{i,j} \exp \left(i \frac{\hbar}{2} \Delta_m^{ij} \partial n_i \partial e_j \right) (e_m n_m) \cdots (e_1 n_1) \\ &= \prod_{i,j} \left(1 + i \frac{\hbar}{2} \Delta_m^{ij} \partial n_i \partial e_j \right) (e_m n_m) \cdots (e_1 n_1) \\ &= \prod_{i < j} \left(1 - i \frac{\hbar}{2} \partial e_i \partial n_j \right) \prod_{i > j} \left(1 + i \frac{\hbar}{2} \partial e_i \partial n_j \right) (e_m n_m) \cdots (e_1 n_1) \\ &= \prod_{i < j} \left(1 + \frac{\hbar^2}{4} \partial n_i \partial e_i \partial n_j \partial e_j \right) (e_m n_m) \cdots (e_1 n_1). \end{aligned}$$

Now replace everything in terms of the harmonic oscillator $T_i = ie_i n_i$ to get

$$\begin{aligned} (*T)^m &= \prod_{i < j} \left(1 - \frac{\hbar^2}{4} \partial T_i \partial T_j \right) T_m T_{m-1} \cdots T_1 \\ &= \sum_{k=0}^t T^{m-2k} (-\hbar^2/4)^k A_k \end{aligned}$$

where A_k is the number of ways of choosing k pairs from among m objects, and t is the integer part of $m/2$. We eventually see that

$$(*T)^m = \sum_{k=0}^t T^{m-2k} (-\hbar^2/8)^k \frac{n!}{(n-2k)!} \quad (15)$$

which is most conveniently written as follows

$$(*T)^n = \exp\left(-\frac{\hbar^2}{8}\partial_{TT}^2\right)T^n. \quad (16)$$

We can now express the Weyl symbol of the product of m Weyl symbols of harmonic oscillators, in terms of the Weyl symbol of the product of m harmonic oscillators. However we cannot use this directly to complete the calculation of the spectrum. The identity (16) must be inverted to give T^m in terms of $(*T)^k$. Starting with

$$T^m = \sum_{g=0}^t \alpha_g (*T)^{m-2g} (-\hbar^2/8)^g$$

where the α_g are constants to be determined, and replacing each $(*T)^k$ using (15), we find that after a little rearrangement

$$T^m = \sum_{k=0}^t T^{n-2k} (-\hbar^2/8)^k \frac{1}{(n-2k)!} \left(\sum_{g=0}^k \alpha_g (n-2g)! \right).$$

The solutions α_g are given by

$$\begin{aligned} \alpha_g &= 1 & g &= 0 \\ &= -m(m-1) & g &= 1 \\ &= 0 & g &> 1. \end{aligned}$$

The inverse of (16) is, therefore,

$$T^m = (*T)^m - \frac{m(m-1)}{8} (*T)^{m-2} \hbar^2$$

or, alternatively,

$$T^m = \left(1 - \frac{\hbar^2}{8}\partial_{*T}^2\right) (*T)^m. \quad (17)$$

We have just established that, in the case of non-resonant Hamiltonians, the wavefunctions of H_h are given by (12), and that the spectrum is given not by (13), but by the following deformation of (13):

$$\left[\prod_{k=0}^{k=d} \left(1 - \frac{\hbar^2}{8}\partial_{T_k}^2\right) \right] H_h(T_1, \dots, T_d)$$

where each $T_k = \hbar(n_k + \frac{1}{2})$, and $n_k \in \mathcal{Z}^+$. To illustrate this the spectrum of T^2 is given, not by $[\hbar(n + \frac{1}{2})]^2$, but by $[\hbar^2(n + \frac{1}{2})^2 - \hbar^2/4]$.

4.2. Resonant Hamiltonians

In this case $K(H^2)$ contains extra terms of the form $e^\Delta T^k, n^\Delta T^k$. The wavefunctions in (12) are no longer wavefunctions for T^h . Nevertheless the corresponding operators can always be diagonalized within the N -eigenspace defined by the span of Ψ_{n_1, \dots, n_d} where n_k satisfy

$$\sum_{k=0}^d \omega_k(n_k + \tfrac{1}{2}) = N. \quad (18)$$

Each N -eigenspace is finite, and so the diagonalization means manipulating only finite matrices. Once more a problem arises as regards finding the spectrum of H_h from the spectrum of the T_k . The extra terms are of course Weyl-ordered and it is desirable to express these in the form $e^\Delta * (*T)^k$, and $n^\Delta * (*T)^k$. In this case we can use identities such as

$$e^\Delta * (*T)^k \phi^n = e^\Delta [\hbar\omega(n + \tfrac{1}{2})]^k \phi^n = [\hbar\omega(n + \tfrac{1}{2})]^k e^\Delta \phi^n \quad (19)$$

to make diagonalization in the N -eigenspaces as painless as possible. We outline the calculation for $e^\Delta T^m$; the calculation for $n^\Delta T^m$ is almost identical.

In the e, n representation, the commutation relations are provided by $[e, n] = \hbar$ etc. The term 'standard ordering' means an ordering of the operators in which the e factors lie to the left of the n factors. In this case the operations which map Weyl-ordered symbols onto the corresponding standard-ordered symbols, and *vice versa*, are provided respectively by

$$\sigma_W^{\text{st}} = \exp\left(-\frac{\hbar}{2}\partial e \cdot \partial n\right) \quad \text{and} \quad \sigma_{\text{st}}^W = \exp\left(\frac{\hbar}{2}\partial e \cdot \partial n\right). \quad (20)$$

It can be shown that for arbitrary Weyl symbols $g(e, n)$

$$g(e, n) = e^\Delta * [\sigma_{\text{st}}^W e^{-\Delta} \sigma_W^{\text{st}} g(e, n)].$$

In particular we look at the case where $g(e, n) = e^\Delta T^k = e^{\Delta+k} n^k i^k$. We find that

$$\begin{aligned} e^\Delta T^k &= e^\Delta * [\sigma_{\text{st}}^W e^{-\Delta} \sigma_W^{\text{st}} e^{\delta+k} n^k i^k] \\ &= e^\Delta * \left[\exp\left(\frac{\hbar}{2}\partial e \cdot \partial n\right) e^{-\Delta} \exp\left(-\frac{\hbar}{2}\partial e \cdot \partial n\right) e^{m+\Delta} n^m i^m \right] \\ &= e^\Delta * \left[\exp\left(\frac{\hbar}{2}\partial e \cdot \partial n\right) e^{-\Delta} \left(e - \frac{\hbar}{2}\partial n\right)^{m+\Delta} n^m i^m \right] \\ &= e^\Delta * \left[\left(e + \frac{\hbar}{2}\partial n\right)^{-\Delta} e^{m+\Delta} n^m i^m \right] \\ &= e^\Delta * \left[\left(1 + \frac{\hbar}{2e}\partial n\right)^{-\Delta} (ien)^m \right]. \end{aligned} \quad (21)$$

Since $T = ien$ we can replace $e^{-1}\partial n$ with $i\partial T$ to get

$$e^\Delta T^k = e^\Delta * \left[\left(1 + i\frac{\hbar}{2}\partial T\right)^{-\Delta} T^k \right]. \quad (22)$$

A similar calculation reveals that

$$n^{\Delta} T^k = n^{-\Delta} * \left(1 - i \frac{\hbar}{2} \partial T\right)^{-\Delta} T^k. \quad (23)$$

As an example of how this might be used, note that $eT^2 = e * T^2 + i\hbar e * T - \hbar^2/2e$. From (11) and (18) we see that

$$eT^2\psi_n = [\hbar^2(n + \frac{1}{2})^2 + i\hbar^2(n + \frac{1}{2}) - \frac{3}{4}\hbar^2] e\psi_n.$$

5. Examples

The harmonic part of the quantum Hamiltonian is used to approximate the original system. It is a perfectly good integrable system in itself and in some sense represents the behaviour of the non-integrable system for a certain range of energies. To illustrate what we have done we look at the case of a well known and well studied non-integrable system, the Hénon-Heiles system [28]. This is represented by the following four-parameter set of Hamiltonians.

$$\frac{m_1}{2}(p_1^2 + q_1^2) + \frac{m_2}{2}(p_2^2 + q_2^2) + \lambda q_2(q_1^2 + \eta q_2^2). \quad (24)$$

5.1. The non-resonant case

The general form of the normal form for a non-resonant Hamiltonian with two degrees of freedom is as follows:

$$H = H^2 + H^4 + H^6 + \dots$$

where

$$H^n = \sum_{2(i+j+k)=n} g_{ij2k} T_1^i T_2^j \hbar^{2k}.$$

Immediately we see that $g_{100} = m_1$, $g_{010} = m_2$, the coefficients of the harmonic oscillator terms. The g_{ijk} are all real numbers determined by the method outlined in section 3. The g_{ij0} coincide exactly with those obtained by the classical method. To order six only three new terms arise, g_{002} , g_{102} and g_{012} . The spectrum of the normal truncated Hamiltonian can be calculated according to (18) for the non-resonant case:

$$E_{n_1 n_2} = \hbar E_{n_1 n_2}^1 + \hbar^2 E_{n_1 n_2}^2 + \hbar^3 E_{n_1 n_2}^3 + \dots \quad (25)$$

where

$$E_{n_1 n_2}^1 = m_1 \left(n_1 + \frac{1}{2}\right) + m_2 \left(n_2 + \frac{1}{2}\right)$$

$$E_{n_1 n_2}^2 = g_{200} \left(n_1 + \frac{1}{2}\right)^2 + g_{110} \left(n_1 + \frac{1}{2}\right) \left(n_2 + \frac{1}{2}\right) + g_{020} \left(n_2 + \frac{1}{2}\right)^2 \\ + (g_{002} - \frac{1}{4}g_{200} - \frac{1}{4}g_{020})^\dagger$$

$$E_{n_1 n_2}^3 = g_{300} \left(n_1 + \frac{1}{2}\right)^3 + g_{210} \left(n_1 + \frac{1}{2}\right)^2 \left(n_2 + \frac{1}{2}\right) \\ + g_{120} \left(n_1 + \frac{1}{2}\right) \left(n_2 + \frac{1}{2}\right)^2 + g_{030} \left(n_2 + \frac{1}{2}\right)^3 \\ + (g_{102} - \frac{3}{4}g_{300} - \frac{1}{4}g_{120}) \left(n_1 + \frac{1}{2}\right)^\dagger \\ + (g_{012} - \frac{3}{4}g_{030} - \frac{1}{4}g_{210}) \left(n_2 + \frac{1}{2}\right)^\dagger.$$

The daggers indicate those terms which are new.

We now turn to the case of a non-resonant Hénon-Heiles system. In table 1 we compare the results for $m_1 = 1.3$, $m_2 = 0.7$ and $\lambda = -0.1$, $\eta = 0.1$, using our method, with the exact results of Noid which were reported by Swimm and Delos in [10]. The results are accurate to within less than 1%. The normal form for the energies is an asymptotic expansion, this feature is identifiable in the progression from the second-order to the eighth-order calculations for the energy. The best results are obtained using the sixth-order approximation for the Hamiltonian. It is with these values we calculate the relative error. The normal form for the Hamiltonian is given by $H_h = H^2 + H^4 + H^6 + H^8$ where

$$H^2 = 1.3T_1 + 0.7T_2$$

$$H^4 = -0.00686375T_1^2 - 0.00843244T_1T_2 - 0.00053571T_2^2 + 0.00199669\hbar^2$$

$$H^6 = -0.00009548T_1^3 - 0.00022941T_1^2T_2 - 0.00012071T_1T_2^2 - 0.00000128T_2^3 \\ + 0.00012994T_1\hbar^2 + 0.00008148T_2\hbar^2$$

$$H^8 = -0.00000164T_1^4 + 0.00000656T_1^3T_2 - 0.00000735T_1^2T_2^2 - 0.00000015T_1T_2^3 \\ - 0.0000000T_2^4 - 0.0000018T_1^2\hbar^2 + 0.00001284T_1T_2\hbar^2 + 0.00000141T_2^2\hbar^2 \\ - 0.00000015\hbar^4.$$

Table 1.

| q-numbers | | Order of normal form | | | | Exact | % rel error |
|-----------|-------|----------------------|--------|--------|--------|--------|-------------|
| n_1 | n_2 | 2nd | 4th | 6th | 8th | | |
| 0 | 0 | 0.1 | 0.9961 | 0.9960 | 0.9961 | 0.9955 | -0.05 |
| 0 | 1 | 1.7 | 1.6909 | 1.6905 | 1.6907 | 1.6870 | -0.23 |
| 1 | 0 | 2.3 | 2.2782 | 2.2774 | 2.2776 | 2.2781 | -0.004 |
| 0 | 2 | 2.4 | 2.3845 | 2.3839 | 2.3841 | 2.3750 | -0.38 |
| 1 | 1 | 3.0 | 2.9645 | 2.9628 | 2.9630 | 2.9584 | -0.15 |
| 0 | 3 | 3.1 | 3.0771 | 3.0761 | 3.0762 | 3.0596 | -0.54 |
| 2 | 0 | 3.6 | 3.5465 | 3.5441 | 3.5442 | 3.5479 | +0.11 |
| 1 | 2 | 3.7 | 3.6497 | 3.6469 | 3.6470 | 3.6347 | -0.34 |
| 2 | 1 | 4.4 | 4.2244 | 4.2200 | 4.2201 | 4.2162 | -0.09 |
| 3 | 0 | 4.9 | 4.8011 | 4.7953 | 4.7953 | 4.8043 | +0.19 |

5.2. The resonant case

In the resonant case more terms arise of the form $K^n + K^{*n}$. For example if $m_1 = m_2 = 1$, we have

$$K = ie_1n_2 \quad K^* = ie_2n_1$$

and the normal form is given by $H = H^2 + H^4 + H^6 + \dots$, where this time

$$H^n = \sum_{2(i+j+k+l)=n} g_{ijk2l} (K^i + K^{*i}) T_1^j T_2^k \hbar^{2l}.$$

To order six, four terms arise which were not present in the classical method. These are the coefficients g_{0002} , g_{0012} , g_{0102} and g_{1002} . We now turn to the case of a resonant Hénon-Heiles Hamiltonian taking $m_1 = m_2 = 1$, $\lambda = 1/10$, and $\eta = -1/3$. In table 2 our calculations of the spectrum are compared with the exact results as calculated by Robnik [9], and the fourth-order normal form calculation done using the old method. $N(18)$, is just the sum of the two small q -numbers $n_1 + n_2 + 1$, and corresponds to the sum of the energies of the uncoupled harmonic oscillators in the lowest order. The normal form to order eight is given by $H = H^2 + H^4 + H^6 + H^8$ where

$$H^2 = T_1 + T_2$$

$$H^4 = -0.00416667T_1^2 + 0.00333333T_1T_2 - 0.00416667T_2^2 \\ - 0.00583333(K^2 + K^{*2}) + 0.00222222\hbar^2$$

$$H^6 = 0.00002338T_1^3 - 0.00040625T_1^2T_2 + 0.00029375T_1T_2^2 - 0.0000544T_2^3 \\ - 0.0001118T_1(K^2 + K^{*2}) + 0.00012153T_2(K^2 + K^{*2}) \\ + 0.0000412T_1\hbar^2 + 0.0000412T_2\hbar^2$$

$$H^8 = -0.00000086T_1^4 + 0.00000452T_1^3T_2 - 0.00000334T_1^2T_2^2 \\ + 0.00000029T_1T_2^3 - 0.00000034T_2^4 - 0.00000161T_1^2(K^2 + K^{*2}) \\ + 0.00000143T_1T_2(K^2 + K^{*2}) - 0.0000032T_2^2(K^2 + K^{*2}) \\ + 0.00000183T_1^2\hbar^2 - 0.00000154T_1T_2\hbar^2 + 0.00000183T_2^2\hbar^2 \\ - 0.00000156(K^4 + K^{*4}) + 0.0000026(K^2 + K^{*2})\hbar^2 - 0.00000026\hbar^4.$$

Table 2.

| N | Order of normal form | | | | Exact | Robnik |
|---|----------------------|--------|--------|--------|--------|--------|
| | 2nd | 4th | 6th | 8th | | |
| 1 | 1 | 0.9989 | 0.9989 | 0.9989 | 0.9989 | 0.9989 |
| 2 | 2 | 1.9922 | 1.9921 | 1.9921 | 1.9921 | 1.9921 |
| | 2 | 1.9922 | 1.9921 | 1.9921 | 1.9921 | 1.9921 |
| 3 | 3 | 2.9889 | 2.9884 | 2.9884 | 2.9884 | 2.9888 |
| | 3 | 2.9889 | 2.9884 | 2.9884 | 2.9884 | 2.9888 |
| | 3 | 2.9655 | 2.9651 | 2.9651 | 2.9651 | 2.9654 |

6. Conclusion

By carrying out the calculation for the normal form to arbitrary high order we get an infinite series which represents the original system in some way. An important question which arises is that of the convergence of the series. It was demonstrated by Siegel [29] that the classical series has a zero radius of convergence if the original system is non-integrable. If it is integrable it will converge for a certain range of the energy. This is perfectly reasonable since a non-integrable system cannot be made integrable

by a simple change of variables. The normal form expansion for the Hamiltonian is itself an integrable system, and its relationship to the original non-integrable one is, at best, asymptotic. An analogous situation holds for the quantum method of normal forms. The asymptotic nature of the expressions for the energy is particularly evident in the first example where the best approximation for the energy levels is given by the sixth-order normal form, and the approximation deteriorates as the order increases.

In the energy calculations we have done, there is little difference between the two approaches, the semi classical approach of Robnik [9], and the 'proper quantum analogue' we have just described. The latter we believe is more transparent and conceptually simpler than the classical method of normal forms. The problem of 'small divisors' which arises in the classical approach, and which leads to difficulties in the treatment of resonant systems does not arise, and the problems associated with the ordering of operators and the commutation of canonical transformations with quantization have been resolved. Having constructed the proper quantum analogue of the method of normal forms we have effectively completed Robnik's programme for developing a purely algebraic method for the quantization of non-integrable classical Hamiltonian systems about a point of stable equilibrium.

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