The Programs for Normalization and Quantization of Polynomial Hamiltonians

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Abstract. We present program GITAN for symbolic computation of the class of polynomial Hamiltonians and formal integrals with the help of ordinary and inverse Birkhoff–Gustavson normalization based on the algorithm ANFER using a conventional pseudocode. The corresponding algorithm of the program QUANTGIT for a semiclassical quantization of the BGNF is described too. Typical examples for a hydrogen atom in external fields demonstrating the runs of the above algorithms and programs as input and output data are given. A comparison of the obtained semiclassical spectrum and its quantum counterpart calculated by the POINTFIELD program is shown.

1 Introduction

In recent papers, a Computer Algebra algorithm for generation of a parametric class of polynomial Hamiltonians which are reduced to the same Birkhoff–Gustavson normal form (BGNF)[1–3] named ANFER (*A*lgorithm of *N*ormal *F*orm *E*xpansion and *R*estoration) has been developed to study the two-dimensional integrable systems [4–7]. Such a type of algorithms and programs have indeed an important application in the BGNF study of both around integrable systems [8–15], geometrical quantization approaches [16–18], algebraic perturbation methods [19–25], and solving applied problems of atomic and laser physics [26–29].

The aim of this talk is to give a unified description using a conventional pseudocode for the algorithms and routines developed by us for generating the class of polynomial Hamiltonians and formal integrals of motion with the help of ordinary[2, 3] and inverse normalization [6]. These algorithms have been implemented by parts in our previous programs GITA [30], GITA^{-1} [31] and ANFER [4, 5], and accumulated here within the framework of the program GITAN. This program is based on an extension of the two-dimensional GITA program for an ordinary normalization till the n-dimensional version and a basic idea of the ANFER algorithm about using the third-type generation function classified by [32] with arbitrary coefficients from a range of the diagonal shift operator on each kth step of the inverse iteration procedure [4]. For extraction of the representative samples of a class of the integrable two-dimensional systems the program BDIC has been developed [7, 33]. The routines of semiclassical quantizing of normal forms [20, 34] using algebraic perturbation theory (APT) algorithm described in [35, 36] have also been incorporated in the the program QUANTGIT presented here as a kernel program surrounded by the specialized procedures tuning on a solution of the specific quantum-mechanical tasks [34, 35, 37]. The programs under consideration are oriented to a support of computer modelling of dynamic and atomic system in external fields like [26–28] and the laser induced formation of Saturnian Hydrogen atoms in a low density plasma [29].

Section 2 gives a brief background of the ordinary and inverse normalization and describes the basic procedures of the program GITAN. The corresponding examples of input and output data of the GITAN run within the framework of a polynomial version BGNF transformation of two- and three-dimensional hydrogen atom in electric F and magnetic γ fields are considered. In Section 3 we display the background and the main procedure of the program QUANTGIT and examine it on a semiclassical quantization of 2D hydrogen atom in the field of distant charge. We also give a comparison of the semiclassical results with one of a pure quantum mechanical algebraic calculation by the program POINTFIELD [35]. In conclusion we discuss the perspective of the development approach to build up new normalization and

quantization procedures. The proposed algorithms and programs GITAN and QUANTGIT have been implemented with the help of REDUCE 3.7[1].

2 Description of Program GITAN

In this section, we review very briefly the ordinary and inverse problems of the BGNF expansion following [3, 4, 6] and the basic procedures `Normform`, `Integral` and `Invert` of the program GITAN for constructing the BGNF and formal integrals of motion, respectively. Consider the Hamiltonian system with n degrees of freedom in the phase space $\Re^n \times \Re^n$, which admits a stable equilibrium point in both non-resonance and most general resonance cases: with incommensurable and commensurable frequencies ω_ν, $(\nu = 1, ..., n)$. Without loss of generality, such an equilibrium point can be put at the origin of the phase space. So, the Hamiltonian $H_{[\delta]}$ of such a system is assumed to be expanded into a formal power series, up to degree s_{max}. As a result, it becomes a polynomial in $(q,\ p)$ of the form

$$H_{[\delta]}(q,p) = \frac{1}{2}\sum_{\nu=1}^{n}\omega_\nu\left(p_\nu^2+q_\nu^2\right) + \sum_{k=3}^{s_{max}} H_{[\delta]}^{(k)}(q,p), \tag{1}$$

where $H_{[\delta]}^{(k)}$ $(k = 3, 4, \cdots)$ denotes the homogeneous part of degree k, while an auxiliary subscript δ equalling 0 or 1 designates what a type of the ordinary or inverse normalization can be chosen as input data for the GITAN algorithm.

The ordinary normalization problem is the conversion of given $H_{[\delta]} = K$ at $\delta = 0$ into a BGNF power series through a local canonical transformation, $(q, p) \to (\xi, \eta)$, which is associated with a type-2 generating function $W_{[\delta]}(q, \eta)$ at $\delta = 0$ of the 'old' position variables q and the 'new' momentum ones η [32]

$$W_{[0]}(q,\eta) = \sum_{\nu=1}^{n} q_\nu\eta_\nu + \sum_{k=3}^{s_{max}} W_{[0]}^{(k)}(q,\eta). \tag{2}$$

On choosing $W_{[0]}(q, \eta) = W(q, \eta)$ suitably, the input $H_{[0]}(q, p)$ is converted to the power series, say output $\Gamma_{[0]}(\xi, \eta) = \Gamma(\xi, \eta)$, through

$$\Gamma_{[0]}(\frac{\partial W_{[0]}}{\partial\eta},\eta) = H_{[0]}(q,\frac{\partial W_{[0]}}{\partial q}), \quad \Gamma_{[0]}(\xi,\eta) = \frac{1}{2}\sum_{\nu=1}^{n}\omega_\nu\left(\eta_\nu^2+\xi_\nu^2\right) + \sum_{k=3}^{s_{max}}\Gamma_{[0]}^{(k)}(\xi,\eta), \tag{3}$$

where every homogeneous part $\Gamma_{[0]}^{(k)}(\xi, \eta)$ $(k = 3, 4, \cdots, s_{max})$ satisfies the Poisson-commuting relation,

$$\left\{\frac{1}{2}\sum_{\nu=1}^{n}\omega_\nu\left(\eta_\nu^2+\xi_\nu^2\right), \Gamma_{[\delta]}^{(k)}(\xi,\eta)\right\} = \left(\sum_{\nu=1}^{n}\omega_\nu\left(\xi_\nu\frac{\partial}{\partial\eta_\nu} - \eta_\nu\frac{\partial}{\partial\xi_\nu}\right)\right)\Gamma_{[\delta]}^{(k)}(\xi,\eta) = 0, \tag{4}$$

which has been rewritten with help of the differential shift operator $D_{\xi,\eta}$ in the form $D_{\xi,\eta}\Gamma_{[\delta]}^{(k)}(\xi, \eta) = 0$.

The inverse problem is extracting a class of the output Hamiltonians $H_{[\delta]} = H$ at $\delta = 1$ which must transform to the previous BGNF output, $\Gamma_{[0]} \equiv \Gamma = \Gamma_{[1]}$ from (3), such as $H_{[1]} \equiv H \supset K \equiv H_{[0]}$ [4, 6].

Let us consider $W_{[1]} \equiv S(q, \eta) \supset -W(q, \eta) \equiv -W_{[0]}$ (see (2)) as the non-normal type-3 generating function of the 'new' position variables q and the 'old' momentum ones η [32],

$$W_{[1]}(q,\eta) = -\sum_{\nu=1}^{n}\eta_\nu q_\nu - \sum_{k=3}^{s_{max}} W_{[1]}^{(k)}(q,\eta), \tag{5}$$

associated with the inverse canonical transformation, $(\xi, \eta) \to (q, p)$, through the relation

$$H_{[1]}(q,-\frac{\partial W_{[1]}}{\partial q}) = \Gamma_{[1]}(-\frac{\partial W_{[1]}}{\partial\eta},\eta), \quad H_{[1]}(q,p) = \frac{1}{2}\sum_{\nu=1}^{n}\omega_\nu\left(p_\nu^2+q_\nu^2\right) + \sum_{k=3}^{s_{max}} H_{[1]}^{(k)}(q,p), \tag{6}$$

where the input BGNF Hamiltonian $\Gamma_{[1]} = \Gamma$ stays in the r.h.s. of Eq. (6) like the ordinary one K in the r.h.s. of Eq. (3). Both $-S$ and W are assumed further to satisfy

$$-S,\ W \in \text{image}D_{q,\eta} \quad \text{with} \quad D_{q,\eta} = \sum_{\nu=1}^{n}\omega_\nu\left(q_\nu\frac{\partial}{\partial\eta_\nu} - \eta_\nu\frac{\partial}{\partial q_\nu}\right). \tag{7}$$

[1] The authors are now implementing the same procedure GITAN in Maple 7.

2.1 Procedure Normform

Input:
δ: for the ordinary problem $\delta = 0$, for the inverse problem $\delta = 1$;
n is the number of degrees of freedom;
s_{max} is the order of the normalization;
ω_ν are frequencies; `r` is the number of resonance frequencies;
$j_{max} \geq 3$ is a maximum degree of terms $H^{(j)}$ of an input Hamiltonian $H_{[0]}$ at $\delta = 0$ or $\Gamma_{[1]}$ at $\delta = 1$;
$H^{(j)}$ are the homogeneous polynomials of degree j in the Cartesian coordinates $(q, p) \in \mathbf{R^n} \times \mathbf{R^n}$;
Output: $W^{(s)}$ are the terms of a generation function W;
$\Gamma^{(s)}$ are the terms of an output Hamiltonian $\Gamma_{[0]}$ at $\delta = 0$ or $H_{[1]}$ at $\delta = 1$;
Local:
$\nu = 1, ..., n$, $s = 3, ..., s_{max}$, $j = 3, ..., s_{max}$;
$k = (k_1, k_2, ..., k_n)$ is multiindex:
$|k| = k_1 + k_2 + ... + k_n$, $k! = k_1!k_2!...k_n!$, $q^k = q_1^{k_1} q_2^{k_2} ... q_n^{k_n}$, $\eta^k = \eta_1^{k_1} \eta_2^{k_2} ... \eta_n^{k_n}$, ...;
x_ν, y_ν, are auxiliary complex coordinates;
$H_{lm}^{(s)}$, $\Gamma_{lm}^{(s)}$, $W_{lm}^{(s)}$ are auxiliary coefficients;
$l = (l_1, l_2, ..., l_n)$, $m = (m_1, m_2, ..., m_n)$ are multiindices;
$c_{lm}^{(s)}$: if $\delta = 0$ then $c_{lm}^{(s)} \equiv 0$ else $c_{lm}^{(s)}$ are arbitrary complex constants;
Global:
$c^{(s)}$: if $\delta = 0$ then $c^{(s)} \equiv 0$ else $c^{(s)} \equiv c^{(s)}(x, y) \in \tilde{R}$ is a complex polynomial of degree s;
q_ν, η_ν, are current coordinates;
Note:
for the ordinary problem ($\delta = 0$) the output Hamiltonian $\Gamma^{(s)}$ is a normal form
1: **for** j:=j_{max} to s_{max} do $H^{(j)} := 0$ end **for**
2: **for** s:=3 to s_{max} do
3: $H^{(s)} := subs(q_\nu \to \frac{1}{\sqrt{2}}(x_\nu + \imath y_\nu),\ \eta_\nu \to \frac{\imath}{\sqrt{2}}(x_\nu - \imath y_\nu),\ H^{(s)})$
4: $H^{(s)} \to \sum\limits_{\substack{l,m \\ |l|+|m|=s}} H_{lm}^{(s)} \prod\limits_{\nu=1}^{n} x_\nu^{l_\nu} y_\nu^{m_\nu}$; $\quad c^{(s)} \to \sum\limits_{\substack{l,m \\ |l|+|m|=s \\ \Sigma_{\nu=1}^n \omega_\nu(m_\nu - l_\nu) \neq 0}} c_{lm}^{(s)} \prod\limits_{\nu=1}^{n} x_\nu^{l_\nu} y_\nu^{m_\nu}$
5: **for all** $(l,\ m) \in H_{lm}^{(s)} \neq 0 \cup c_{lm}^{(s)} \neq 0$
if $\sum_{\nu=1}^n \omega_\nu(m_\nu - l_\nu) \neq 0$
then $\Gamma_{lm}^{(s)} := c_{lm}^{(s)}$; $\quad W_{lm}^{(s)} := \imath(-1)^\delta (H_{lm}^{(s)} + c_{lm}^{(s)}) \Big[\sum\limits_{\nu=1}^{n} \omega_\nu(m_\nu - l_\nu)\Big]^{-1}$
else $\Gamma_{lm}^{(s)} := H_{lm}^{(s)}$; $\quad W_{lm}^{(s)} := 0$
end **if**
end **for all**
6: $W^{(s)} := \sum\limits_{\substack{l,m \\ |l|+|m|=s}} W_{lm}^{(s)} \prod\limits_{\nu=1}^{n} x_\nu^{l_\nu} y_\nu^{m_\nu}$; $\Gamma^{(s)} := \sum\limits_{\substack{l,m \\ |l|+|m|=s}} \Gamma_{lm}^{(s)} \prod\limits_{\nu=1}^{n} x_\nu^{l_\nu} y_\nu^{m_\nu}$
7: $W^{(s)} := subs(x_\nu \to \frac{1}{\sqrt{2}}(q_\nu - \imath\eta_\nu),\ y_\nu \to \frac{\imath}{\sqrt{2}}(-q_\nu - \imath\eta_\nu),\ W^{(s)})$
$\Gamma^{(s)} := subs(x_\nu \to \frac{1}{\sqrt{2}}(q_\nu - \imath\eta_\nu),\ y_\nu \to \frac{\imath}{\sqrt{2}}(-q_\nu - \imath\eta_\nu),\ \Gamma^{(s)})$
8: **for** j:=$s+1$ to s_{max}

$$\Gamma^{(j)} := H^{(j)} + (-1)^\delta \sum_{\substack{|k|\geq 1 \\ |k|<l<j \\ l=j-(s-2)|k|}} \frac{1}{k!} \left[\Big(\frac{\partial W^{(s)}}{\partial q}\Big)^k \Big(\frac{\partial^{|k|} H^{(l)}}{\partial \eta^k}\Big) - \Big(\frac{\partial W^{(s)}}{\partial \eta}\Big)^k \Big(\frac{\partial^{|k|} \Gamma^{(l)}}{\partial q^k}\Big) \right].$$

end **for**
9: **for** j:=3 to s_{max} do $H^{(j)} := \Gamma^{(j)}$ end **for**
end **for** (2:)
end of procedure `Normform`

The implementation of the above procedure `normform` of reduction to a BGNF depends on a ratio between frequencies ω_ν. Birkhoff has proved [1] that if the frequencies ω_ν of Hamiltonian (1) are incommensurable,

there is a canonical transformation $(q,p) \to (\xi,\eta)$, such that in new coordinates the Hamiltonian $\Gamma_{[0]}(\xi,\eta)$ is the function of n independent integrals of motion $I_\nu = \frac{1}{2}(\xi_\nu^2 + \eta_\nu^2)$:

$$H_{[0]}(q,p) \Rightarrow \Gamma_{[0]}(\xi,\eta) = \sum_{\nu=1}^{n} \omega_\nu I_\nu + \sum_{\mu,\nu} \alpha_{\mu\nu} I_\mu I_\nu + \dots . \tag{8}$$

If the frequencies ω_ν are commensurable, i.e. if there exist r resonance relations of the form

$$(B,\omega) = \sum_{\nu=1}^{n} b_{k\nu}\omega_\nu = 0, \qquad k = 1,2,...,r, \tag{9}$$

where matrix $B = \{b_{k\nu}\}$ has integer coefficients $b_{k\nu}$ and rank r, $\omega = \{\omega_1,...,\omega_n\}$ is n-vector, then Hamiltonian (1) cannot be reduced to the form (8). In this case, for BGNF Γ from (3), we have $(n-r)$ independent formal integrals of motion $I^{(2)}_{k'}$ of the form [2]

$$I^{(2)}_{k'} = \sum_{\nu=1}^{n} \frac{a_{\nu k'}}{2}(\xi_\nu^2 + \eta_\nu^2), \qquad \{I^{(2)}_{k'}, \Gamma\} = 0, \qquad k' = 1,2,...,n-r, \tag{10}$$

with coefficients $a_{\nu k'}$ being the solutions of the system of linear algebraic equations

$$(B,A) = \sum_{\nu=1}^{n} b_{k\nu} a_{\nu k'} = 0, \qquad k = 1,2,...,r, \qquad k' = 1,2,...,n-r, \tag{11}$$

where matrix $A = \{a_{\nu k'}\}$ has $n-r$ columns consisting of n-vectors. After the substitution of solutions $a_{\nu k'}$ of the system of equations (11) into the formula (10), with the help of inverse transformation $(\xi,\eta) \to (q,p)$ up to the given order $s_{max}-2$, one can calculate the $(n-r)$ approximate formal integrals of motion $I_{k'}(q,p)$, $k' = \overline{1,n-r}$ for the input Hamiltonian $H_{[0]}$ from (1), i.e. $pb = \{I_{k'}, H_{[0]}\} = 0$, up to the order s_{max}. As input data the frequencies ω and ratios between those given by matrix B of input Hamiltonian from (1), and generating function $W_{[0]}$ calculated by the above procedure `normform` are used here. The corresponding algorithm for the analytical calculation of approximate formal integrals of motion up to the given order s_{max} using an auxiliary construction of some $n-r$ parametric formal integral of motion $I^{(2)} = \sum_{\nu=1}^{n} a_\nu(\eta_\nu^2 + \xi_\nu^2)/2$, with coefficients $a_\nu = a_{\nu k'}$ satisfying (11), i.e. $\{I^{(2)}, \Gamma\} = 0$, as local variables, are implemented by procedures `Integral` and `Invert` of the program GITAN at $\delta = 0$, which are introduced below.

2.2 Procedure Integral

Input:
n is the number of degrees of freedom;
s_{max} is the normalization order;
$H^{(s)}$ are homogeneous parts of degree s of the initial Hamiltonian H in the Cartesian coordinates $(q,p) \in \mathbf{R^n} \times \mathbf{R^n}$;
r is the number of relations between frequencies;
$b_{k\nu}$ are the components of matrix B from (9);
Output:
$I_{k'}$ is the array of formal integrals of motion;
pb is the Poisson bracket;
Local:
$\nu = 1,...,n$, $k = 1,...,r$, $k' = 1,...,n-r$, $s = 2,...,s_{max}$;
I is an auxiliary homogeneous polynomial of second order;
a_ν are auxiliary coefficients;
HH is an auxiliary Hamiltonian
Global:
ξ_ν, η_ν, are coordinates;
$csnt(k')$ are arbitrary coefficients;
z is an auxiliary cutting parameter: $z^s = \{$if $s \le s_{max}$ then z^s else $0\}$.
1: **for** $\nu = 1$ to n do $p_{\nu,2} = zp_{\nu,0}$, $q_{\nu,2} = zq_{\nu,0}$ end **for**

2: **for** $s = 3$ to s_{max} do call **INVERT**(s) end **for**

3: solving of system of equations $\sum_{\nu=1}^{n} b_{k,\nu} a_\nu = 0, k = 1, ..., r: \quad a_\nu \overset{\nu=1,n}{:=} a_\nu(csnt(k'),\ k' = 1, ..., n-r)$

4: $I := \sum_{\nu=1}^{n} \frac{a_\nu}{2}(\eta_\nu^2 + \xi_\nu^2)$

5: $I := subs(\eta_\mu \overset{\mu=1,n}{\to} p_{\mu,s_{max}}, \xi_\mu \overset{\mu=1,n}{\to} q_{\mu,s_{max}},\ I)$

6: $HH := subs(p_\mu \overset{\mu=1,n}{\to} zp_{\mu,0}, q_\mu \overset{\mu=1,n}{\to} zq_{\mu,0}, \sum_{s=2}^{s_{max}} H^{(s)})$

7: $I := subs(p_{\mu,0} \overset{\mu=1,n}{\to} p_\mu, q_{\mu,0} \overset{\mu=1,n}{\to} q_\mu, HH - I)$

8: $pb := \sum_{\nu=1}^{n} \left(\frac{\partial I}{\partial p_\nu} \frac{\partial(\sum_{s=2}^{s_{max}} H^{(s)})}{\partial q_\nu} - \frac{\partial(\sum_{s=2}^{s_{max}} H^{(s)})}{\partial p_\nu} \frac{\partial I}{\partial q_\nu} \right)$

9: **for** $k' = 1$ to $n - r$ do $I_{k'} := subs(z = 1, csnt(k') = 1, csnt(k \neq k') = 0, I)$ end **for**

end of procedure `Integral`

Procedure Invert

Input:

n is the number of degrees of freedom;

s_{max} is the normalization order; s is a current number;

$W^{(s)}$ is the term of a generation function W;

Output:

$(p_{\nu,s},\ q_{\nu,s})$ as a function of $(p_{\nu,s-1},\ q_{\nu,s-1})$

Local:

$\nu, \mu = 1, ..., n$ is the number of degrees of freedom; $x_{\nu,0},\ x_{\nu,1},\ y_\nu$, wt are auxiliary functions;

Global:

z is an auxiliary cutting parameter: $z^s = \{\text{if } s \leq s_{max} \text{ then } z^s \text{ else } 0\}$.

1: **for** $\nu = 1$ to n do wt:=subs$(\eta_\nu \to z\eta_\nu,\ q_\nu \to zq_\nu,\ W^{(s)})$ end **for**

2: **for** $\nu = 1$ to n do $x_{\nu,0} := y_\nu$ end **for**;

3: **for** $\nu = 1$ to n do $x_{\nu,1} := subs(\eta_\mu \overset{\mu=1,n}{\to} \frac{x_{\mu,0}}{z}, x_{\nu,0} - \frac{1}{z}\frac{d\text{wt}}{dq_\nu})$ end **for**

4: **repeat**

for $\nu = 1$ to n do $x_{\nu,0} := x_{\nu,1}$ end **for**

for $\nu = 1$ to n do $x_{\nu,1} := subs(\eta_\mu \overset{\mu=1,n}{\to} \frac{x_{\mu,0}}{z}, x_{\nu,0} - \frac{1}{z}\frac{d\text{wt}}{dq_\nu})$ end **for**

until $\sum_{\nu=1}^{n}(x_{\nu,1} - x_{\nu,0}) \neq 0$

5: **for** $\nu = 1$ to n do

$p_{\nu,s} := subs(q_\mu \overset{\mu=1,n}{\to} \frac{q_{\mu,s-1}}{z},\ y_\mu \overset{\mu=1,n}{\to} \frac{p_{\mu,s-1}}{z}, x_{\nu,0})$;

$q_{\nu,s} := subs(q_\mu \overset{\mu=1,n}{\to} q_{\mu,s-1},\ \eta_\mu \overset{\mu=1,n}{\to} p_{\mu,s-1}, q_\nu + \frac{dW^{(s)}}{d\eta_\nu})$;

end **for**

end of procedure `Invert`

The program GITAN including the above procedures `Normform`, `Integral` and `Invert` has been implemented in REDUCE 3.7. As a set of input data we use the following: the number of degrees of freedom $n \geq 2$, the frequencies ω, r ratios between ω given by matrix B from (9), the input Hamiltonian $H_{[0]}$ from (1), and the normalization order s_{max}. The results of run of the program GITAN for ordinary ($\delta = 0$) and inverse ($\delta = 1$) analytical construction of BGNF and the calculated approximate formal integrals of motion up to the given order s_{max} are displayed below.

3 Examples of Runs of GITAN Program

2D Hydrogen atom We consider the results of calculation of a normal form and approximate integral of motion for a two-dimensional limit of the Saturnian Hydrogen atom (initially confined to the plane $z = 0$ with no velocity component in the z-direction) in a circularly polarized electric field F and magnetic

B fields (in atomic units) [27]

$$\bar{H}_0 = \frac{1}{2}\bar{p}_x^2 + \frac{1}{2}\bar{p}_y^2 - \frac{1}{\sqrt{\bar{x}^2+\bar{y}^2}} + \frac{\omega_c}{2}(-\bar{y}\bar{p}_x + \bar{x}\bar{p}_y) + \frac{\omega_c^2}{8}(\bar{x}^2+\bar{y}^2) + F(\bar{x}\cos\omega_f t + \bar{y}\sin\omega_f t),$$

where $\omega_c = eB/(m_e c)$ is the cyclotron frequency, and ω_f is the electric field frequency. In a synodic frame rotating with the field frequency ω_f,

$$\bar{H}_0 = \bar{K} = \frac{1}{2}\bar{p}_x^2 + \frac{1}{2}\bar{p}_y^2 - \frac{1}{\sqrt{\bar{x}^2+\bar{y}^2}} - (\omega_f - \frac{\omega_c}{2})(-\bar{y}\bar{p}_x + \bar{x}\bar{p}_y) - F\bar{x} + \frac{\omega_c^2}{8}(\bar{x}^2+\bar{y}^2),$$

after scaling coordinates and momenta $x = \omega_c^{2/3}\bar{x},\ y = \omega_c^{2/3}\bar{y},\ p_x = \omega_c^{-1/3}\bar{p}_x,\ p_y = \omega_c^{-1/3}\bar{p}_y$ we find the Hamiltonian

$$H_0 = K = \frac{1}{2}p_x^2 + \frac{1}{2}p_y^2 - \frac{1}{\sqrt{x^2+y^2}} - (\Omega - \frac{1}{2})(-yp_x + xp_y) - \varepsilon x + \frac{1}{8}(x^2+y^2),$$

where $K = \bar{K}{\omega_c}^{-2/3}$, $\Omega = \omega_f\omega_c^{-1}$ and $\varepsilon = F\omega_c^{-4/3}$, K is the Jacobi constant. The corresponding Hamiltonian H in the Levi-Civita variables p, q on the energy manifold determined by $H = \sqrt{2/-K}\sqrt{x^2+y^2}$ apart from the change of time variable $t \to \tau$ with $dt/d\tau = \sqrt{2/-K}$ has the oscillator form [38]

$$H = \sqrt{\frac{2}{-K}} = \frac{1}{2}(p_1^2+p_2^2+q_1^2+q_2^2) + a_1(-q_2p_1+q_1p_2)(q_1^2+q_2^2) + a_2(q_1^2+q_2^2)^3 + b_1(q_1^4-q_2^4), \quad (12)$$

where $b_1 = F\sqrt{-2K}/(8K^2)$, $a_1 = (\Omega - \frac{1}{2})/(-4K)$, $a_2 = 1/(128K^2)$. As a result of executing GITAN at $\delta = 0$, the BGNF $\Gamma = \sum_{k=2}^{s_{max}} \Gamma^{(k)}$ at $s_{max} = 8$ is obtained:

$$\begin{aligned}
&\Gamma^{(2)} = I_1, \quad \Gamma^{(3)} = \Gamma^{(5)} = \Gamma^{(7)} = 0,\\
&\Gamma^{(4)} = \frac{3b_1}{2}I_1I_2 + a_1I_1I_3, \qquad (13)\\
&\Gamma^{(6)} = -\frac{a_1^2}{2}I_1I_3^2 - \frac{7a_1b_1}{2}I_1I_2I_3 + \frac{a_2}{2}(5I_1^3 - 3I_1I_3^2) - \frac{17b_1^2}{16}(I_1^3 + 3I_1I_2^2),\\
&\Gamma^{(8)} = \frac{a_1^3}{2}I_1I_3^3 + \frac{b_1a_1^2}{16}(4I_1^3I_2 + 127I_1I_2I_3^2) + \frac{3}{2}a_1a_2(3I_1I_3^3 - 5I_1^3I_3) + \frac{375b_1^3}{32}(I_1^3I_2 + I_1I_2^3)\\
&\quad + \frac{b_1^2a_1}{16}(12I_1I_3^3 + 315I_1I_2^2I_3 + 107I_1^3I_3) + \frac{3b_1a_2}{8}(-55I_1^3I_2 + 21I_1I_2I_3^2),
\end{aligned}$$

where

$$\begin{aligned}
I_1 &= \frac{1}{2}(\eta_1^2+\eta_2^2+\xi_1^2+\xi_2^2), \qquad I_3 = (\xi_1\eta_2 - \xi_2\eta_1),\\
I_2 &= \frac{1}{2}(\eta_1^2-\eta_2^2+\xi_1^2-\xi_2^2), \qquad I_4 = (\xi_1\xi_2 + \eta_1\eta_2).
\end{aligned}$$

Note that the above normal form representation is not unique with regard for the relation $I_1^2 = I_2^2+I_3^2+I_4^2$.

We are now in a position to give an example to show how the inverse GITAN at $\delta = 1$ is proceeded to BGNF Hamiltonians. We take as the input a BGNF Hamiltonian $\Gamma_{[1]} = \Gamma^{(2)} + \Gamma^{(4)}$ from (13). For example, if we choose the auxiliary homogenous polynomials $c^{(3)} = 0$ and $c^{(4)}$ with arbitrary complex-valued coefficients, then we find that the Hamiltonian $H^{(4)}$ consists of 188 monomials. Therefore, we choose the real polynomial $c^{(4)}$ and extract a class of real-valued Hamiltonians $H = H^{(2)} + H^{(3)} + H^{(4)}$ at $s_{max} = 4$:

$$\begin{aligned}
H^{(2)} &= \frac{1}{2}({p_1}^2 + {p_2}^2 + {q_1}^2 + {q_2}^2), \qquad H^{(3)} = 0,\\
H^{(4)} &= q_2^4(-\frac{1}{3}c^{(4)}_{0,0,2,2} - c^{(4)}_{0,0,0,4} - b_1) - \frac{1}{2}{q_2}^3p_1a_1 + \frac{1}{2}{q_2}^2q_1p_2a_1 + {q_2}^2{p_2}^2c^{(4)}_{0,0,2,2} - \frac{1}{2}q_2{q_1}^2p_1a_1\\
&\quad -\frac{1}{2}q_2{p_2}^2p_1a_1 - \frac{1}{2}q_2{p_1}^3a_1 + {q_1}^4(-\frac{1}{3}c^{(4)}_{2,2,0,0} - c^{(4)}_{0,4,0,0} + b_1) + \frac{1}{2}{q_1}^3p_2a_1 + {q_1}^2{p_1}^2c^{(4)}_{2,2,0,0} \qquad (14)\\
&\quad +\frac{1}{2}q_1{p_2}^3a_1 + \frac{1}{2}q_1p_2{p_1}^2a_1 + {p_2}^4c^{(4)}_{0,0,0,4} + {p_1}^4c^{(4)}_{0,4,0,0}
\end{aligned}$$

Setting $c^{(4)}_{0,4,0,0} = c^{(4)}_{0,0,0,4} = 0$ in Hamiltonian (14) in the case $a_1 = 0$, H becomes [38]

$$H = (q_1^2 c^{(4)}_{2,2,0,0} + \frac{1}{2}){p_1}^2 + (q_2{}^2 c^{(4)}_{0,0,2,2} + \frac{1}{2}){p_2}^2 + \frac{1}{2}{q_1}^2 - (\frac{1}{3}c^{(4)}_{2,2,0,0} - b_1){q_1}^4 + \frac{1}{2}{q_2}^2 - (\frac{1}{3}c^{(4)}_{0,0,2,2} + b_1){q_2}^4.$$

Note that H turns out to be a Hamiltonian of Liouville type, which is well known to admit the separation of variables in its associated Hamilton-Jacobi equation [39]. In such a way it has been shown [6, 7] that if the perturbed harmonic oscillators with a homogeneous cubic-polynomial potential and with a homogeneous quartic-polynomial potential share the same BGNF up to degree four, then the both oscillators satisfy the Bertrand–Darboux integrability conditions (BDIC) [40].

One can indeed examine that for the Hamiltonian H given by (12) at $a_1 = 0$ the second exact integral of motion I in involution with H, i.e. $\{H, I\} = 0$, has the form

$$I = b_1(q_1^2 + p_1^2) - a_2(-q_2 p_1 + q_1 p_2)^2 + 2a_2 b_1 q_1^2 (q_1^2 + q_2^2)^2 + 2b_1^2 q_1^4. \tag{15}$$

Fig. 1 shows the 3D plots of the above exact integral I(a) and the approximate integral I_a(b)-(d) in coordinates $p_2,\ q_2$ calculated by GITAN at $\delta = 0$ till eighth order[2] ($s_{max} = 8$) with fixed K, ω_c, F and three sets of parameters $a_1,\ a_2,\ b_1$. One can see a qualitative agreement in the exact and approximate isolines of Poincaré sections, which can be improved taking into account higher-order calculations($s_{max} \geq 8$) that are needed to describe similar but non-integrable systems having both discrete and continuous spectrum [29]. For the 2D hydrogen atom a further analysis of the above approximate integrals and normal forms connecting convergence to Liouville-integrability can use some approaches in this line [10–15].

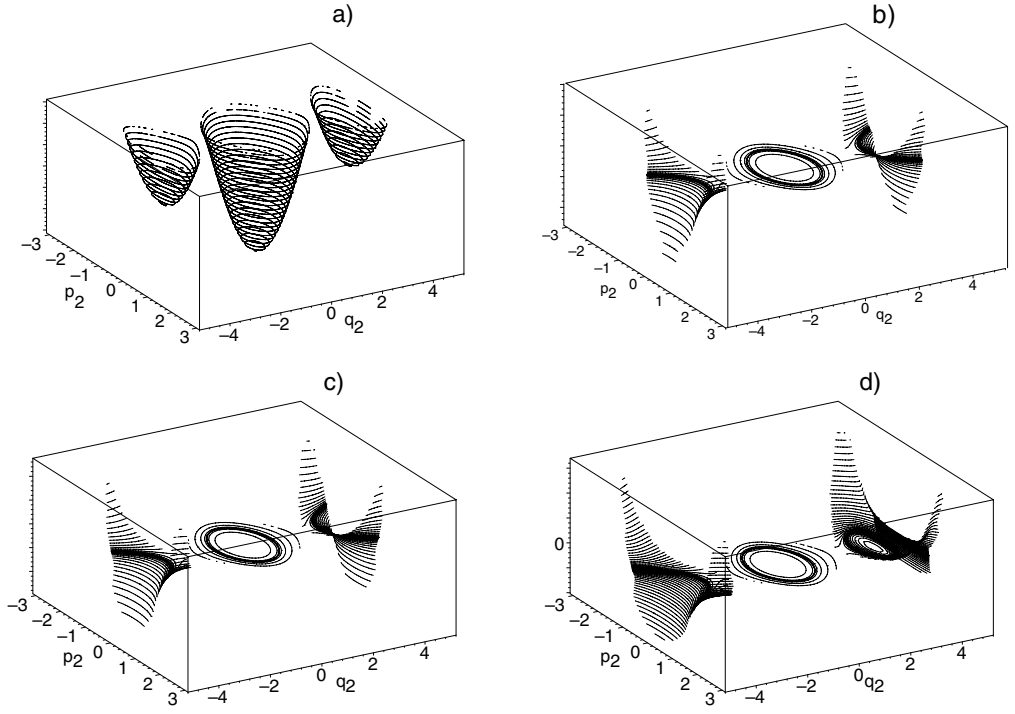

Fig. 1. The 3D plots of the exact integral of motion I and the approximate ones I_a ($s_{max} = 8$) for Hamiltonian (12) at $K = -1.071 \cdot 10^{-3}$, $\omega_c = 1.472 \cdot 10^{-5}$, $F = -3.389 \cdot 10^{-6}$, $b_1 = 6.974 \cdot 10^{-2}$, $a_2 = 2.457 \cdot 10^{-2}$ are displayed in (a) and (b) – (d), respectively. Parameters $\omega_f = 7.36 \cdot 10^{-6}$ and $a_1 = 0$ for (a) and (b), $\omega_f = 8.464 \cdot 10^{-6}$ and $a_1 = 1.051 \cdot 10^{-2}$ for (c), and $\omega_f = 9.936 \cdot 10^{-6}$ and $a_1 = 2.453 \cdot 10^{-2}$ for (d)

3D Hydrogen atom As an example we consider the 3D Hydrogen atom in parallel electric F and magnetic γ fields. In [26] this task has been reduced to a four-dimensional one with a two-parametric

[2] the integral of motion I_a evaluated by GITAN at $s_{max} = 8$ consists of 237 monomials and is not displayed

Hamiltonian

$$H = \frac{1}{2}\sum_{j=1}^{4}(q_j^2+p_j^2) - \frac{4F}{\omega^3}(q_1^2+q_2^2+q_3^2+q_4^2)(q_1^2-q_2^2-q_3^2+q_4^2) \\ -\frac{4\gamma}{\omega^4}(q_1^2+q_2^2+q_3^2+q_4^2)(q_1^2+q_4^2)(q_2^2+q_3^2), \tag{16}$$

where $\omega^2 = 4\gamma L_z - 8E$, at a given value of an integral L_z and energy E. With the help of the program GITAN at $\delta = 0$ the BGNF at $s_{max} = 6$ is obtained, but is displayed here till $s_{max} = 4$[3]:

$$\Gamma^{(2)} = \frac{1}{2}\sum_{j=1}^{4}(\eta_j^2+\xi_j^2), \qquad \Gamma^{(3)} = 0, \tag{17}$$
$$\Gamma^{(4)} = -\frac{3F}{2\omega^3}(\xi_1^2+\xi_4^2+\eta_1^2+\eta_4^2)^2 + \frac{2F}{\omega^3}(\eta_1\xi_4-\eta_4\xi_1)^2 \\ +\frac{3F}{2\omega^3}(\xi_2^2+\xi_3^2+\eta_2^2+\eta_3^2)^2 - \frac{2F}{\omega^3}(\eta_2\xi_3-\eta_3\xi_2)^2.$$

There are 3 resonance relations between frequencies in the Hamiltonian (17): $\omega_1 = \omega_2 = \omega_3 = \omega_4 = 1$, i.e. $n = 4$, $r = 3$, $n-r = 1$, therefore, there is a single integral of motion in the form (10): $I_1 = \Gamma^{(2)}$. According to transformation $(\xi, \eta) \to (q, p)$ (see the above procedure `Invert`), a rather cumbersome expression for the decomposition of an approximate integral of motion I_1 has been calculated by GITAN at $\delta = 0$, but it is not displayed here[4]. The examination of this integral decomposition by means of testing the Poisson bracket $pb = \{H, I_1\}$ has been evaluated successfully, $pb = 0$, by the procedure `Integral`.

4 Description of Program QUANTGIT

4.1 The Example of Quantization of 2D Hydrogen Atom

Semiclassical quantization schemes of the 2D limit case of the hydrogen atom in magnetic field have been considered in detail in [19, 22, 34]. To illustrate the run of our program QUANTGIT for a semiclassical quantization of BGNF and to have a comparison of results with a known quantum spectrum, we consider here the 2D hydrogen atom with the charge Z_a in the electric field of a distant point charge Z_b with Hamiltonian

$$H = \frac{1}{2}(p_1^2+p_2^2+q_1^2+q_2^2) + \frac{1}{2}(-2E)^{-3/2}(q_1^4-q_2^4)\frac{Z_b}{R^2} \\ -\frac{1}{4}(-2E)^{-2}(q_1^2+q_2^2)(q_2^4-4q_1^2q_2^2+q_1^4)\frac{Z_b}{R^3}+..., \tag{18}$$

where R is a distance between charges Z_a and Z_b, at a fixed value of energy $E < 0$. As a result of executing of GITAN, the BGNF, $\Gamma = \sum_{k=2}^{s_{max}}\Gamma^{(k)}$, at $s_{max} = 10$ has been calculated. We present only a few expressions[5]

$$\Gamma^{(2)} = \frac{1}{2}(\eta_1^2+\eta_2^2+\xi_1^2+\xi_2^2),$$
$$\Gamma^{(4)} = \frac{Z_b}{R^2}(-2E)^{-3/2}\frac{3}{16}f((\eta_1^2+\xi_1^2)^2-(\eta_2^2+\xi_2^2)^2), \tag{19}$$
$$\Gamma^{(6)} = -\frac{1}{64}(-2E)^{-2}({\xi_2}^2+{\xi_1}^2+{\eta_1}^2+{\eta_2}^2)[5({\xi_2}^2+{\eta_2}^2)^2+5({\xi_1}^2+{\eta_1}^2)^2 - \\ -8({\xi_1}^2+{\eta_1}^2)({\xi_2}^2+{\eta_2}^2)-12(\eta_1\eta_2+\xi_1\xi_2)^2]\frac{Z_b}{R^3} \\ -\frac{17}{128}(-2E)^{-3}(({\xi_1}^2+{\eta_1}^2)^3+({\xi_2}^2+{\eta_2}^2)^3)\frac{{Z_b}^2}{R^4}.$$

[3] $\Gamma^{(6)}$ consists of 169 monomials

[4] the correction for integral of motion I at $s_{max} = 6$ consists of 190 monomials

[5] the corrections $\Gamma^{(8)}$ and $\Gamma^{(10)}$ consist of 35 and 190 monomials, the corrections $\Gamma^{(k)}$ at odd k are equal to zero

Each even term $G(2\kappa)$ is here a sum of homogeneous polynomials $G_j(2\kappa)$ of order 2κ, i.e. $G(2\kappa) = \sum_{j=\kappa}^{2\kappa-2} R^{-j} G_j(2\kappa)$. The program QUANTGIT converts a normal form in the complex variables $z_k = \frac{1}{\sqrt{2}}(\eta_k + i\xi_k)$, $z_k^* = \frac{1}{\sqrt{2}}(\eta_k - i\xi_k)$ and with the help of the Weyl substitution

$$z_k^m z_k^{*n} \longrightarrow \frac{1}{2^m} \sum_{l=0}^{m} \frac{m!}{l!(m-l)!} \hat{a}_k^{+l} \hat{a}_k^n \hat{a}_k^{+\,m-l}, \qquad [a_k, a_l^+] = \delta_{kl}, \tag{20}$$

transforms it to the quantum BGNF in terms of the operators $a,\ a^+$. Then the eigenvalue problem

$$\Gamma|\lambda\rangle = \lambda(E)|\lambda\rangle \tag{21}$$

concerning the spectral parameter $\lambda(E)$ is solved by using the eigenvector definition:

$$|k_1, k_2\rangle = (\sqrt{k_1! k_2!})^{-1} (\hat{a}_1^+)^{k_1} (\hat{a}_2^+)^{k_2} |0,0\rangle, \qquad \hat{a}_1|0,0\rangle = \hat{a}_2|0,0\rangle = 0,$$

where $k_1, k_2 = 0, 1, 2, ...$ are the oscillator quantum numbers. For solving the eigenvalue problem (21) we expand the Hamiltonian Γ in the sum $\Gamma = \sum P_j R^{-j}$, where $P_j = \sum_{\kappa=[j/2]-1}^{j} G_j(2\kappa)$. An action of operator P_j on eigenvector $|k_1, k_2\rangle$ has the form $P_j|k_1, k_2\rangle = \sum_{\kappa=-[(j-1)/2]}^{[(j-1)/2]} \alpha_{2\kappa} |k_1 - 2\kappa, k_2 + 2\kappa\rangle$. Decomposing the eigenvector $|\lambda\rangle$ by basis $|k_1, k_2\rangle$, we have:

$$\begin{aligned}\lambda(E) = k_1 + k_2 + 1 + \frac{3Z_b}{4R^2}(-2E)^{-3/2}(k_1 + k_2 + 1)(k_1 - k_2) \\ -\frac{Z_b}{8R^3}(-2E)^{-3/2}(k_1 + k_2 + 1)(5(k_1 - k_2)^2 - 4k_1k_2 - 2k_1 - 2k_2 + 3) + ...\end{aligned}$$

To calculate the energy $E < 0$ in parabolic quantum numbers $n_1, n_2 = 0, 1, 2, ...$ we will use the substitution $k_1 = 2n_1$, $k_2 = 2n_2$. The quasi classical spectrum of energy $E = E_{n_1,n_2}$ of the problem (18) is calculated from the algebraic equation $\lambda(E) = Z_a\sqrt{-2/E}$ with the aid of a standard iteration routine

$$\begin{aligned}E_{n_1,n_2} = -\frac{Z_a^2}{2n^2} + \frac{3Z_b}{2Z_aR^2}nd + \frac{n^2Z_b}{2Z_a^2R^3}(n^2 - 6d^2 - 1) \\ -\frac{n^4Z_b^2}{64Z_a^4R^4}(68n^2 - 12d^2 + 85) - \frac{n^3dZ_b}{64Z_a^3R^4}(156n^2 - 436d^2 - 227) + ...,\end{aligned} \tag{22}$$

where $n = n_1 + n_2 + 1/2$, $d = n_1 - n_2$. The above algorithm has been realized with procedures [35, 36] as part of program QUANTGIT. In [35] the energy spectrum for 2D Hydrogen atom has been calculated by an ordinary algebraic perturbation theory method with the help of program POINTFIELD[6]

$$\begin{aligned}E^e_{n_1,n_2} = -\frac{Z_a^2}{2n^2} + \frac{3Z_b}{2Z_aR^2}nd + \frac{n^2Z_b}{2Z_a^2R^3}(n^2 - 6d^2 - 1) \\ -\frac{n^4Z_b^2}{64Z_a^4R^4}(68n^2 - 12d^2 + 67) - \frac{n^3dZ_b}{64Z_a^3R^4}(156n^2 - 436d^2 - 227) + ...\end{aligned} \tag{23}$$

One can see that a difference between these relations is only in the free terms in the brackets, which is a consequence of the known arbitrariness in the quasi classical correspondence rules. We examined that the Weyl substitution (20) realized in the basic procedure `Quantconvert` of the program QUANTGIT provides a minimal difference in the above results as compared to the symmetrized or the Iordan ones. Note the quasi classical formulas give a better description of an upper part of the spectrum as compared with the pure quantum perturbation ones. Below we present the procedure `Quantconvert` only.

4.2 Procedure Quantconvert

Input: n is the number of degrees of freedom;
s_{max} is the normalization order;
ω_ν are frequencies;
$\Gamma^{(s)}$ are the terms of a BGNF Γ;

[6] We do not allow the constant term $Z_a(Z_b - 1)/R$.

Output:
$\hat{\Gamma}^{(s)}$ are the terms of a quantum BGNF operator;
$G^{(s)}$ are the actions of operator $\Gamma^{(s)}$ by eigenfunctions $|k_1, k_2, ..., k_n\rangle$ of operator $\hat{\Gamma}^{(2)}$;
Local:
$\nu = 1, ..., n$ is the number of degrees of freedom;
$z_\nu,\ z^*_\nu$, are auxiliary variables;
$l,\ m,\ m'$ are the parameters of the Weyl transformation;
Global:
$\xi_\nu,\ \eta_\nu$, are current coordinates and momenta;
$\hat{a}^+_\nu,\ \hat{a}_\nu$ are creation and annihilation operators;
$|k_1, k_2, ..., k_n\rangle$ are the eigenfunctions of harmonic oscillator $\hat{\Gamma}^{(2)}$;
k_ν are quantum numbers;
1: **for** s:=3 to s_{max} do
2: $\quad \Gamma^{(s)} := subs(\eta_\nu \to \dfrac{1}{\sqrt{2}}(z_\nu + z^*_\nu),\ \xi_\nu \to \dfrac{1}{\sqrt{2}}(z_\nu + z^*_\nu),\quad \Gamma^{(s)})$
3: $\quad \hat{\Gamma}^{(s)} := subs(z^m_\nu z^{*m'}_\nu \to \dfrac{1}{2^m}\displaystyle\sum_{l=0}^{m} \frac{m!}{l!(m-l)!}\hat{a}^{+\,l}_\nu \hat{a}^{m'}_\nu \hat{a}^{+\,m-l}_\nu,\ \Gamma^{(s)})$
4: $\quad G^{(s)} := \hat{\Gamma}^{(s)}|k_1, k_2, ..., k_n\rangle$
5: $\quad$ **while** $G^{(s)} \supset \hat{a},\ \hat{a}^+$ do
$\qquad G^{(s)} := subs(\hat{a}^+_\nu|\ , k_\nu,\ \rangle \to \sqrt{k_\nu + 1}|\ , k_\nu + 1,\ \rangle, \hat{a}_\nu|\ , k_\nu,\ \rangle \to \sqrt{k_\nu}|\ , k_\nu - 1,\ \rangle, G^{(s)})$
$\quad$ end **while**
end **for**(1:)
end of procedure `Quantconvert`

5 Conclusion

We have demonstrated the efficiency of the proposed recursive symbolic algorithm GITAN for the generation of both ordinary and inverse BGNF and formal integrals of motion as well as the calculation of perturbation series by means of algorithm QUANTGIT, which are needed to solve the specific applied problems in atomic and laser physics [29, 28]. Developing such an approach with the quantization procedures [34] similar to the normal form perturbation method [24] and polynomial Lie algebra to [25] is in line of our interest too.

The further long write-up of GITAN program, the development of its algorithm based on Lie transformations [8, 9] and corresponding comparison are beyond the subject of this talk and will be published elsewhere.

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