A Comparison of Algorithms for the Normalization and Quantization of Polynomial Hamiltonians

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Abstract—Algorithms and programs for the normalization of polynomial Hamiltonians of classical mechanics by the Birkhoff–Gustavson and Deprit–Hori, as well as quasi-classical quantization procedures for normal forms, are compared. The algorithms and programs are represented in a universal pseudocode and implemented in the computer algebra systems REDUCE, MAPLE, and MATHEMATICA. Examples that illustrate the operation of these algorithms and programs for polynomial Hamiltonians of atomic systems in external electromagnetic fields are considered.

1. INTRODUCTION

Algorithms for reducing the classical Hamiltonian to the normal form and the subsequent quantization are widely used for the integration and analysis of classical and quantum equations of motion [1, 2]. Since the Hamiltonian of a hydrogen-like atom is related to the Hamiltonian of the harmonic oscillator by the Levi–Civita transform [3], the method of normal form quantization is also applied for the calculation of characteristics of atomic systems in external fields [4, 5]. By way of example, we consider the calculation of the quasi-classical spectrum of a two-dimensional hydrogen atom in the electric field of a distant point charge and compare the result with the spectrum of the quantum problem [6].

The application of various computer algebra systems significantly extends the capabilities of various implementations of normalization procedures [7–9]. Therefore, the representation of such algorithms in a universal pseudocode and their comparison is important for the evaluation of their efficiency and implementation [10].

In this paper, we compare algorithms for reducing the class of polynomial Hamiltonians (anharmonic oscillators) to the normal form by the Birkhoff–Gustavson method and Lie transformations (the Deprit–Hori method); we also compare procedures for finding an approximate integral of motion and constructing a quantum analog of the normal form. The procedures are represented in a pseudocode. Examples that illustrate the operation of these algorithms and programs for polynomial Hamiltonians of atomic systems in external electromagnetic fields are considered. The algorithms are implemented in REDUCE, MAPLE, and MATHEMATICA.

2. NORMALIZATION PROCEDURE

Consider algorithms for the construction of the Birkhoff–Gustavson normal form [11] for Hamiltonians that can be represented in the polynomial form in the vicinity of an equilibrium point in the phase space $(p^{(0)}, q^{(0)}) \in R^n \times R^n$:

$$H(q, p) = H^{(2)}(q, p) + \sum_{j=3}^{j_{\max}} H^{(j)}(q, p), \tag{1}$$

$$H^{(2)}(q, p) = \sum_{\nu=1}^{n} \frac{\omega_\nu}{2}(p_\nu^2 + q_\nu^2), \tag{2}$$

$$H^{(j)}(q, p) = \sum_{|l|+|m|=j} V_{lm} q^l p^m. \tag{3}$$

The normalization procedure consists of finding the new Hamiltonian

$$\Gamma(\xi, \eta) = \sum_{\nu=1}^{n} \frac{\omega_\nu}{2}(\eta_\nu^2 + \xi_\nu^2) + \sum_{s=3}^{s_{\max}} \Gamma^{(s)}(\xi, \eta) \tag{4}$$

and the canonical transformation $(q, p) \leftarrow (\xi, \eta)$ that relates Hamiltonians (1) and (4). Here, $\Gamma^{(s)}(\xi, \eta)$ are homogeneous polynomials of degree s that satisfy the following relation, which involves the Poisson brackets $\{,\}$:

$$\left\{\sum_{\nu=1}^{n} \frac{\omega_\nu}{2}(\eta_\nu^2 + \xi_\nu^2), \Gamma^{(s)}(\xi, \eta)\right\} = \left(\sum_{\nu=1}^{n} \omega_\nu\left(\xi_\nu \frac{\partial}{\partial \eta_\nu} - \eta_\nu \frac{\partial}{\partial \xi_\nu}\right)\right)\Gamma^{(s)}(\xi, \eta) = 0. \tag{5}$$

Depending of the definition of the canonical transformation $(q, p) \longrightarrow (\xi, \eta)$, there are several methods for obtaining normal forms [1].

The Birkhoff–Gustavson (BG) method [11] is based on the representation of old momenta p and new coordinates ξ in terms of the new momenta η and old coordinates q as

$$p_\nu = \frac{\partial W_{BG}}{\partial q_\nu}, \quad \xi_\nu = \frac{\partial W_{BG}}{\partial \eta_\nu} \tag{6}$$

using the generating function of the second type

$$W_{\mathrm{BG}}(q, \eta) = \sum_{\nu=1}^{n} q_\nu \eta_\nu + \sum_{s=3}^{s_{\max}} W_{\mathrm{BG}}^{(s)}(q, \eta). \tag{7}$$

The Deprit–Hori (DH) method [12, 13] is based on the representation of old canonical variables (q, p) in terms of the new variables (ξ, η):[1]

$$\begin{aligned} q_\nu &= \xi_\nu + \sum_{k=1}^{s_{\max}-2} \frac{1}{k!} L_W^k \xi_\nu, \\ p_\nu &= \eta_\nu + \sum_{k=1}^{s_{\max}-2} \frac{1}{k!} L_W^k \eta_\nu. \end{aligned} \tag{8}$$

For this purpose, the generator

$$W_{\mathrm{DH}}(\xi, \eta) = \sum_{k=3}^{s_{\max}} W_{\mathrm{DH}}^{(k)}(\xi, \eta) \tag{9}$$

is used. Here, the operator L_W^k is defined by the recurrence $L_W^k = \mathrm{L}_W(L_W^{k-1})$, $L_W^0 = 1$ in terms of the Lie differential operator

$$L_W f \equiv L(f, W) = \{f, W\}. \tag{10}$$

Substituting series (6) or (8) into the basic equation

$$H(q, p) = \Gamma(\xi, \eta),$$

expanding the left-hand and right-hand sides in the Taylor series in powers of the canonical variables (q, η) or (ξ, η), and separating homogeneous polynomials of degrees $s = 3, 4, \ldots, s_{\max}$ of these variables, we obtain the system of equations

$$\Gamma^{(s)} = \{\Gamma^{(2)}, W^{(s)}\} + H^{(s)} + T_s, \tag{11}$$

which can be solved sequentially beginning with $s = 3$. In Eq. (11), the unknowns are the components of the new Hamiltonian $\Gamma^{(s)}$ and the components of the generating function $W_{\mathrm{BG}}^{(s)} = W^{(s)}$ or of the generator $W_{\mathrm{DH}}^{(s)} = W^{(s)}$. The auxiliary polynomials T_s depend on the components $\Gamma^{(s')}$, $W^{(s')}$, and $H^{(s')}$, which are determined earlier. Here, $s' = 3, \ldots, s-1$ and $T_3 \equiv 0$.

The Birkhoff–Gustavson algorithm with the generating function (7) was described in [10] in terms of a universal pseudocode. Here, we present a pseudocode for finding the normal forms (11) by the Deprit–Hori method with the generator (9).

Algorithm 1

Input:

n is the number of degrees of freedom;

$s_{\max}$ is the order of normalization;

ω_ν are the frequencies;

$H^{(s)}$ are the homogeneous polynomials of degree s of the initial Hamiltonian.

Output:

$W^{(s)}$ are the homogeneous polynomials of degree s of the generating function;

$G^{(s)}$ are the homogeneous polynomials of degree s of the Hamiltonian to be found.

Local:

$\nu = 1, \ldots, n$ is the index of a degree of freedom;

$s = 3, \ldots, s_{\max}$ is the step number of the normalization procedure;

$k = (k_1, k_2, \ldots, k_n)$ is a multindex;

$|k| = k_1 + k_2 + \ldots + k_n$, $l = (l_1, l_2, \ldots, l_n)$,

$q^k = q_1^{k_1} q_2^{k_2} \ldots q_n^{k_n}$, $p^k = p_1^{k_1} p_2^{k_2} \ldots p_n^{k_n}$, …;

x_ν and y_ν are auxiliary coordinates;

$H_{lm}^{(s)}$, $\Gamma_{lm}^{(s)}$, and $W_{lm}^{(s)}$ are auxiliary coefficients;

$l = (l_1, l_2, \ldots, l_n)$, $m = (m_1, m_2, \ldots, m_n)$.

Global:

q_ν and p_ν are the current coordinates and momenta.

Functions:

$$L(f, W^{(j)}) = \sum_\nu \left(\frac{\partial f}{\partial q_\nu} \frac{\partial W^{(j)}}{\partial p_\nu} - \frac{\partial f}{\partial p_\nu} \frac{\partial W^{(j)}}{\partial q_\nu} \right);$$

$$K_{j,i} = \frac{1}{j} \sum_{m=2}^{i} L(K_{j-1, i-m+2}, W^{(m+1)});$$

$$K_{1,i} = \sum_{m=2}^{i} L(h_{i+2-m}, W^{(m+1)}); \; K_{0,i} = K^{(i)}.$$

procedure

for $s := 3$ **to** $s_{\max}$ **do**

$$1: T_s := \sum_{i=2}^{s-2} L(H_{s-i+1}, W^{(i+1)}) + \sum_{i=4}^{s} K_{i-2, s-i+2}$$

$$2: t^{(s)} := subs\left(q_\nu \longrightarrow \frac{x_\nu - \imath y_\nu}{\sqrt{2}}, p_\nu \longrightarrow \frac{y_\nu - \imath x_\nu}{\sqrt{2}}, \right.$$

[1] The equivalence of the methods proposed in [12, 13] was established in [14].

$H^{(s)} + T_s\Big)$

3: $t^{(s)} \longrightarrow \sum_{l,\,m:\ |l|+|m|\,=\,s} t_{lm}^{(s)} x^l y^m$;

4: **for all** $(l, m) \in t_{lm}^{(s)} \neq 0$

if $\omega m - \omega l \neq 0$

then begin $G_{lm}^{(s)} := 0$;

$$W_{lm}^{s} := \frac{-\imath(t_{lm}^{(s)} + G_{lm}^{(s)})}{\omega m - \omega l}$$

end

else begin $G_{lm}^{(s)} := t_{lm}^{(s)}$; $W_{lm}^{(s)} := 0$

end

end if

end for all

5: $W^{(s)} := \sum_{l,\,m:\ |l|+|m|\,=\,s} W_{lm}^{(s)} x^l y^m$;

$$G^{(s)} := \sum_{l,\,m:\ |l|+|m|\,=\,s} G_{lm}^{(s)} x^l y^m$$

6: $W^{(s)} := subs\Big(x_\nu \longrightarrow \frac{q_\nu + \imath p_\nu}{\sqrt{2}},$

$y_\nu \longrightarrow \frac{p_\nu + \imath q_\nu}{\sqrt{2}}, W^{(s)}\Big)$

$G^{(s)} := subs\Big(x_\nu \longrightarrow \frac{q_\nu + \imath p_\nu}{\sqrt{2}},$

$y_\nu \longrightarrow \frac{p_\nu + \imath q_\nu}{\sqrt{2}}, G^{(s)}\Big)$

end for

end of procedure

This procedure involves the following sequence of steps.

Step 1. Finding the auxiliary polynomial T_s. In contrast to Steps 2–6, it is specific for the Deprit–Hori method.

Steps 2–3. Switching to the auxiliary variables (x, y) and finding the coefficients of the polynomial T_s.

Step 4. Solution of Eq. (11). The selection of the auxiliary variables (x, y) is caused by the fact that the monomial $x^l y^m$ is an eigenfunction of the normal form operator. If the corresponding eigenvalue is nonzero (the branch *then*), we have a single equation with two unknown coefficients $W_{lm}^{(s)}$ and $G_{lm}^{(s)}$. When calculating the normal form,[2] we set $G_{lm}^{(s)} = 0$ and solve this equation in $W_{lm}^{(s)}$. If the corresponding eigenvalue is zero (the branch *else*), we calculate the coefficient $G_{lm}^{(s)}$ (while setting the corresponding coefficient $W_{lm}^{(s)}$ to zero).

Steps 5–6. Constructing the polynomials $W^{(s)}$ and $G^{(s)}$ and changing to the coordinates (q, p).

The efficiency of Algorithm 1 implemented in various computer algebra systems is illustrated in Table 1. This table presents the number of monomials *NM*, the computation time (in seconds) of the normal form G and the generator W_{DH} up the given order $s_{\max}$ for the following polynomial Hamiltonians H.

Table 1

1	Example	1	2	3	4
2	$s_{\max}$	40	4	4	6
3	*NMH*	3	5	8	26
4	*NMG*	230	14	46	200
5	NMW_{BG}	209	22	590	164
6	NMW_{DH}	209	17	410	164
	Time T	s	s	s	s
7	*BG*(*mws*)	89.1	2.0	54.2	7.9
8	*DH*(*mws*)	25.4	1.3	29.6	5.1
9	*BG*(*nb*)	16.4	2.1	16.2	4.6
10	*DH*(*nb*)	20.9	1.1	3.8	2.0
11	*BG*(*red*) [10]	90.5	0.2	78.8	3.0
12	*DH*(*red*)	18.5	0.2	18.2	2.8
13	*DH*(*red*) [7]	106.0	0.3	2.3	8.2

Example 1.

$$H(q, p) = \frac{1}{2}(p_1^2 + q_1^2) + a_1 q_1^4.$$

Example 2.

$$H(q, p) = \frac{\omega_1}{2}(p_1^2 + q_1^2) + \frac{\omega_2}{2}(p_2^2 + q_2^2) + a q_1^2 q_2.$$

Example 3.

$$H(q, p) = \sum_{\nu=1}^{3} \frac{\omega_\nu}{2}(p_\nu^2 + q_\nu^2) + \alpha q_1 q_3^2 + \beta q_2 q_3^2.$$

[2] When solving other problems, for example, when reconstructing the class of polynomial Hamiltonians that can be reduced to the given normal form by canonical transformations [10], the coefficients $G_{lm}^{(s)} = c_{lm}^{(s)}$ are arbitrary complex constants $c_{lm}^{(s)} \in Z$.

Example 4.

$$H = \frac{1}{2}\sum_{j=1}^{4}(q_j^2 + p_j^2)$$

$$-\frac{4F}{\omega^3}(q_1^2+q_2^2+q_3^2+q_4^2)(q_1^2-q_2^2-q_3^2+q_4^2)$$

$$-\frac{4\gamma}{\omega^4}(q_1^2+q_2^2+q_3^2+q_4^2)(q_1^2+q_4^2)(q_2^2+q_3^2).$$

Row 1 of Table 1 contains the number of the example, and row 2 shows the order of normalization $s_{\max}$. Rows 3–6 show the number of monomials (NM) involved in the initial Hamiltonian H, in the normal form G, in the generating function W_{BG} (7), and in the generator W_{DH} (9). Rows 7–12 show the execution time of the normalization procedure (in seconds) on a Pentium-III based computer with 600 MHz 128 MByte RAM under Windows 98. The procedure was based on the Birkhoff–Gustavson (BG) and Deprit–Hori (DH) methods, which were implemented in REDUCE (red), MAPLE (mws), and MATHEMATICA (nb). Row 13 shows the execution time of the program described in [7]. In that program, monomials are sequentially subtracted from the component $H^{(s)}$ of the Hamiltonian represented in terms of the initial variables (with account for Step 1) until this component vanishes, and Steps 2, 4, and 6 of Algorithm 1 are applied to each of these monomials. In our implementation of Algorithm 1, the list of coefficients $t_{lm}^{(s)}$ is composed before executing Step 4, and Step 4 is applied to each of these coefficients. In the first case, the memory is saved, while the number of operations is saved in the second case.

When the algorithm is implemented, the greatest saving of the computation time is obtained when expressions are fully expanded (which is done by the operator expand in MAPLE and MATHEMATICA). When other operators are used for simplifying algebraic expressions (simplify, collect, etc.), a significant part of the computation time is spent on reducing these expressions to the form that is required by the interpreter of the system.

It is seen from Table 1 that the computation time significantly increases when the frequencies are specified as incommensurable parameters (examples 2 and 3) compared to an explicit specification of the frequencies (examples 1 and 4). This is because intermediate algebraic expressions involve rational fractions with polynomial denominators. The expansion of such expressions is most efficient in MATHEMATICA.

The computation time also depends on specific features of the interpreter and on the structure of the components of the Hamiltonian $H^{(s)}$ ($s \geq 3$). In example 1, the computation by the BG method in MATHEMATICA is by a factor of 1.3 faster than the computation by the DH method in MATHEMATICA; however, the computation by the BG method in REDUCE is by a factor of 4.9 slower than the computation by the DH method in REDUCE. In example 2, we see the converse situation.

Remark. To reduce the number of operations (due to substitutions), it is reasonable to switch to the complex variables at step 2 before executing the main loop (on the variable s) of Algorithm 1, which requires the corresponding redefinition of the function L.

3. INTEGRALS OF MOTION

One advantage of the Deprit–Hori method is in the explicit algorithm that transforms an arbitrary function f from one canonical variables (q, p or ξ, η) to the other for the given generator $W \equiv W_{\mathrm{DH}}$:

$$f(q_\nu, p_\nu) = f(\xi_\nu, \eta_\nu) + \sum_{k=1}^{s_{\max}-2}\frac{1}{k!}L_W^k f(\xi_\nu, \eta_\nu),$$

$$f(\xi_\nu, \eta_\nu) = f(q_\nu, p_\nu) + \sum_{k=1}^{s_{\max}-2}\frac{(-1)^k}{k!}L_W^k f(q_\nu, p_\nu).$$

The corresponding algorithm is presented in the pseudocode.

Algorithm 2

Input:

δ : 1 denotes that the function given in the old variables is to be represented in terms of the new variables (direct change)

–1 denotes that the function given in the new variables is to be represented in terms of the old variables (inverse change)

$f_0(q_\nu, p_\nu)$ is the function represented in terms of the initial variables.

Output:

$f_1(q_\nu, p_\nu)$ is the function represented in terms of the desired variables.

Comment: The definition of the global functions L and $W^{(s)}$ are given in Algorithm 1.

1: **for** $s := 3$ **to** $s_{\max}$ **do**

$d_1^{(s)} := L(f_0(q_\nu, p_\nu), W^{(s)})$

end for

2: **for** $j := 2$ **to** $s_{\max} - 2$ **do**

for $s := 3$ **to** $s_{\max}$ **do**

$$d_j^{(s)} := \sum_{t=3}^{s-1} L(d_{j-1}^{(s+2-t)}, W^{(t)})$$

end for

end for

3: **for** $s := 3$ **to** $s_{\max}$ **do**

$$f_1^{(s)}(q_\nu, p_\nu) = \sum_{j=1}^{s_{\max}-2} \frac{\delta^j d_j^{(s)}}{j!}$$

end for

$$4: f_1(q_\nu, p_\nu) = f_0(q_\nu, p_\nu) + \sum_{s=3}^{s_{\max}} f_1^{(s)}(q_\nu, p_\nu).$$

Substituting the coordinates q_ν and momenta p_ν for $f_0(q_\nu, p_\nu)$, we obtain a procedure for deriving an explicit relation between the old and new coordinates and momenta.

Remark. In the implementation of the algorithms, we use the same notation for the old and new variables in order to reduce the number of operations (due to substitutions).

The same procedure is used to find approximate integrals of motion. To this end, we use the Gustavson proposition (see [11]): for the system with n degrees of freedom and r resonance relations

$$\sum_{\nu=1}^{n} b_{k,\nu}\omega_\nu = 0, \quad k = 1, \ldots, r, \tag{12}$$

there exists an $(n - r)$-parametric integral of motion, which can be calculated by the following algorithm.

Algorithm 3

Input:

n is the number of degrees of freedom;

r is the number of resonance relations;

$b_{k\nu}$ are the elements of matrix (12).

Output:

I is the integral of motion.

Local:

$\nu = 1, \ldots, n$ is the index of a degree of freedom;

$k = 1, \ldots, r$ is the index of a resonance relation;

eqs is the auxiliary system of equations;

sol is the solution to system *eqs*.

Global:

ξ_η and η_ν are the coordinates and momenta;

a_ν are auxiliary variables.

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

$$2: eqs := list\left(\sum_{\nu=1}^{n} b_{k,\nu}a_\nu = 0, k = 1, \ldots, r\right)$$

$$3: sol := (a_1, \ldots, a_n) = solve(eqs, (a_1, \ldots, a_n))$$

$$4: I := subs(sol, I)$$

Substituting the result produced by Algorithm 3 at the input of Algorithm 2 for the function $f_0(q_\nu, p_\nu)$ (for $\delta = -1$), we find an approximate integral of motion for the given Hamiltonian H. To compare the efficiency of Algorithm 2 based on different methods and implementations, we present in Table 2 the computation time T (in seconds) and the number of monomials *NMI* of the approximate integral of motion I; the other notation is the same as in Table 1.

Table 2

Example	2	3	4
NMI_{DH}	75	2120	198
Time T	s	s	s
$DH(mws)$	1.3	–	0.2
$DH(nb)$	0.8	7.3	0.4
$DH(red)$	0.1	6.1	0.6

4. QUANTIZATION PROCEDURE

The procedure of quasi-classical quantization reduces the normal form (4) to the quantum normal form

$$\hat{\Gamma}(a^+, a) = \sum_{s=2}^{s_{\max}} \hat{\Gamma}^{(s)}(a^+, a) \tag{13}$$

using the Weyl transformation $(p, q) \longrightarrow (a^+, a)$ [15]. The quantum normal form is represented in terms of the production and annihilation operators a_ν^+, a_ν, $[a_\nu^+, a_\mu] = \delta_{\mu\nu}$ $(\mu, \nu = 1, 2, \ldots, n)$. This procedure also finds the result of the action

$$G = \sum_{s=2}^{s_{\max}} G^{(s)} \equiv \hat{\Gamma}(a^+, a)|k_1, k_2, \ldots, k_n\rangle,$$
$$G^{(s)} = \hat{\Gamma}^{(s)}(a^+, a)|k_1, k_2, \ldots, k_n\rangle \tag{14}$$

of the resulting quantum normal form on the basis of the n-dimensional harmonic oscillator $|k_1, k_2, \ldots, k_n\rangle$. The corresponding algorithm of the quasi-classical normal form quantization is written in the pseudocode.

Algorithm 4

Input:

n is the number of degrees of freedom;

$s_{\max}$ is the order of normalization;

ω_ν are the frequencies;

$\Gamma^{(s)}$ are the components of the normal form.

Output:

$\hat{\Gamma}^{(s)}$ are the components of the quantum normal form;

$G^{(s)}$ are the actions of the components of the normal form operator $\Gamma^{(s)}$ on the eigenfunction $|k_1, k_2, \ldots, k_n\rangle$ of the operator $\hat{\Gamma}^{(2)}$.

Local:

$\nu = 1, \ldots, n$ is the index of a degree of freedom;

z_ν and z_ν^* are auxiliary variables;

l, m, and m' are the parameters of the Weyl transformation.

Global:

ξ_ν and η_ν are the coordinates and momenta;

a_ν^+ and a_ν are the production and annihilation operators; $|k_1, k_2, \ldots, k_n\rangle$ are the basis functions of the n-dimensional harmonic oscillator;

k_ν are the quantum numbers.

1: **for** s: = 3 **to** $s_{\max}$ **do**

$$2: \Gamma^{(s)} := subs\left(\eta_\nu \longrightarrow \frac{1}{\sqrt{2}}(z_\nu + z_\nu^*),\right.$$

$$\left.\xi_\nu \longrightarrow \frac{1}{\sqrt{2}}(z_\nu + z_\nu^*), \Gamma^{(s)}\right)$$

$$3: \hat{\Gamma}^{(s)} := subs\left(z_\nu^m z_\nu^{*m'}\right.$$

$$\left.\longrightarrow \frac{1}{2^m}\sum_{l=0}^{m}\frac{m!}{l!(m-l)!}\hat{a}_\nu^{+l}\hat{a}_\nu^{m'}\hat{a}_\nu^{+m-l}, \Gamma^{(s)}\right)$$

4: $G^{(s)} := \hat{\Gamma}^{(s)}|k_1, k_2, \ldots, k_n\rangle$

5: **while** $G^{(s)} \supset a, a^+$ **do**

$G^{(s)} := subs$

$(a_\nu^+|, k_\nu, \rangle \longrightarrow \sqrt{k_\nu + 1}|, k_\nu + 1, \rangle$

$a_\nu|, k_\nu, \rangle \longrightarrow \sqrt{k_\nu}|, k_\nu - 1, \rangle, G^{(s)})$

end while

end for (1:)

The results produced by Algorithm 4 are used to solve the eigenvalue problem

$$\hat{\Gamma}|\lambda\rangle = \lambda(E)|\lambda\rangle. \tag{15}$$

By way of example, consider the Hamiltonian of the two-dimensional hydrogen atom ($n = 2$) with the charge Z_a in the electric field of a distant point charge Z_b for a fixed $E < 0$:

$$H = \frac{1}{2}(p_1^2 + p_2^2 + q_1^2 + q_2^2) + \frac{Z_b(-2E)^{-3/2}}{2R^2}(q_1^4 - q_2^4) - \frac{Z_b(-2E)^{-2}}{4R^3}(q_1^2 + q_2^2)(q_2^4 - 4q_1^2q_2^2 + q_1^4) + \ldots, \tag{16}$$

where $\varepsilon = R^{-1} \ll 1$ is the reciprocal of the distance between the charges Z_a and Z_b. Algorithm 1 produced the Birkhoff–Gustavson normal form (4). For $s_{\max} = 8$, all odd-order terms of this form vanish. Here are the first two nonzero terms:

$$\Gamma^{(2)} = \frac{1}{2}(\eta_1^2 + \eta_2^2 + \xi_1^2 + \xi_2^2),$$
$$\Gamma^{(4)} = \frac{3Z_b(-2E)^{-3/2}}{16R^2}((\eta_1^2 + \xi_1^2)^2 - (\eta_2^2 + \xi_2^2)^2). \tag{17}$$

Using Algorithm 4, we find the result of the action of the normal form on the eigenfunction of the two-dimensional harmonic oscillator ($|k_1, k_2\rangle$):

$$\begin{aligned} G &= \hat{\Gamma}|k_1, k_2\rangle \\ &= (a_1^+a_1 + a_2^+a_2 + 1)|k_1, k_2\rangle \\ &\quad - \frac{3Z_b(-2E)^{-3/2}}{4R^2}(a_1^{+2}a_1^2 + 2a_1^+a_1 \\ &\quad - a_2^{+2}a_2^2 - 2a_2^+a_2)|k_1, k_2\rangle + \ldots \\ &= (k_1 + k_2 + 1)|k_1, k_2\rangle \\ &\quad - \frac{3Z_b(-2E)^{-3/2}}{4R^2}(k_1 + k_2 + 1)(k_1 - k_2)|k_1, k_2\rangle \\ &\quad - \frac{3Z_b(-2E)^{-2}}{8R^3}(k_1 + k_2 + 1) \\ &\quad \times\sqrt{(k_1^2 - k_1)(k_2^2 + 3k_2 + 2)}|k_1 - 2, k_2 + 2\rangle \\ &\quad - \frac{3Z_b(-2E)^{-2}}{8R^3}(k_1 + k_2 + 1) \\ &\quad \times\sqrt{(k_1^2 + 3k_1 + 2)(k_2^2 - k_2)}|k_1 + 2, k_2 - 2\rangle + \ldots. \end{aligned}$$

To solve the eigenvalue problem (15), we represent in the form of series the action G of the normal form operator $\hat{\Gamma}$ on the vector $|k_2, k_2\rangle$

$$G = (k_1 + k_2 + 1)|k_1, k_2\rangle + \sum_{j=1}^{j_m} R^{-j}\sum_{a=-j+1}^{j-1} f_{k_1+a, k_2-a}^{(j)}|k_1 + a, k_2 - a\rangle, \tag{18}$$

the desired eigenvector

$$|\lambda\rangle = \sum_{j=0}^{j_m-1} R^{-j}\sum_{a=-j+1}^{j-1} b_{k_1+a, k_2-a}^{(j)}|k_1 + a, k_2 - a\rangle, \tag{19}$$

and the spectral parameter

$$\lambda(E) = \sum_{j=0}^{j_m} R^{-j}\lambda^{(j)}. \tag{20}$$

To find the coefficients $b^{(j)}_{k_1+a,k_2-a}$ and $\lambda^{(j)}$ in the expansions (19) and (20) with the small parameter $\varepsilon = R^{-1}$, we use a fragment of the algorithm for solving the eigenvalue problem (15) in the form of a system of nonhomogeneous algebraic equations [6]:

$$\begin{aligned} f^{(j)}_{k_1,k_2} &= 0 \longrightarrow \lambda^{(j)}, \\ f^{(j)}_{k_1+a,k_2-a} &= 0 \longrightarrow b^{(j-2)}_{k_1+a,k_2-a}, \quad a \neq 0, \end{aligned} \tag{21}$$

with the initial conditions

$$\begin{aligned} b^{(0)}_{k_1,k_2} &= 1, \quad b^{(0)}_{k_1+a,k_2-a} = 0, \quad a \neq 0, \\ \lambda^{(0)} &= k_1 + k_2 + 1. \end{aligned} \tag{22}$$

The quasi-classical spectrum $E_{n,d}$ of the hydrogen atom in the field of a distant point charge is found from the algebraic equation[3]

$$\lambda(E_{n,d}) = Z_a\sqrt{-2/E_{n,d}},$$

where $n = (k_1 + k_2)/2 + 1/2$ and $d = (k_1 - k_2)/2$, using the standard procedure

$$\begin{aligned} E_{n,d} = &-\frac{Z_a^2}{2n^2} + \frac{3Z_b}{2Z_aR^2}nd \\ &+ \frac{n^2Z_b}{2Z_a^2R^3}(n^2 - 6d^2 - 1 + \delta_1^{(3)}) \\ &- \frac{n^3dZ_b}{64Z_a^3R^4}(156n^2 - 436d^2 - 227 + \delta_1^{(4)}) \\ &- \frac{n^4Z_b^2}{64Z_a^4R^4}(68n^2 - 12d^2 + 85 + \delta_2^{(4)}) + \ldots. \end{aligned}$$

Here, $\delta_i^{(j)} \equiv 0$. The spectrum determined in the framework of the quantum-mechanical perturbation theory [6] differs from the quasi-classical spectrum (23) only in the values of $\delta_i^{(j)}$; in particular, $\delta_1^{(3)} = \delta_1^{(4)} = 0$ and $\delta_2^{(4)} = -18$. The total computation time for this example (with *smax* = 10) by Algorithms 1 and 4 and by the fragment of the algorithm for solving the eigenvalue problem (15) implemented in MAPLE is 90 s.

5. CONCLUSIONS

The representation of the normal form depends on the relationship between the frequencies: if the frequencies ω_ν are incommensurable, i.e., the relations $\sum_{\nu=1}^{n} \omega_\nu(m_\nu - l_\nu) = 0$ hold only for $m_\nu = l_\nu$ ($\nu = 1, 2, \ldots, n$), then the Hamiltonian has n independent integrals of motion $I_\nu = (\xi_\nu^2 + \eta_\nu^2)/2$. Then, the action of the corresponding quantum operator $\hat{\Gamma}$ takes the diagonal form $G = \hat{\Gamma}|k_1, k_2, \ldots, k_n\rangle = \gamma|k_1, k_2, \ldots, k_n\rangle$; and for solving the eigenvalue problem (15), it is sufficient to solve the equation $\gamma = \lambda(E)$. In this case, the eigenfunction of the problem coincides with the eigenfunction $|k_1, k_2, \ldots, k_n\rangle$ of the operator $\hat{\Gamma}^{(2)}$. If the frequencies ω_ν are commensurable, then usually not all quantities $I_\nu = (\xi_\nu^2 + \eta_\nu^2)/2$ are integrals of motion, and the action of the normal form operator on the basis of the n-dimensional harmonic oscillator G has a nondiagonal form. Since the initial Hamiltonian involves a small parameter ε (in the example under consideration, $\varepsilon = R^{-1}$), the function G can be expanded in the series

$$G = \left[\sum_{\nu=1}^{n}\left(k_\nu + \frac{1}{2}\right)\right]|k_1, k_2, \ldots, k_n\rangle + \sum_{j=l}^{j_m} G^{(j)}\varepsilon^j,$$

where $l \geq 1$. If $G^{(l)}$ is given in the diagonal representation $G^{(l)} = f_{k_1,\ldots,k_n}|k_1, \ldots, k_n\rangle$, then the eigenfunctions in the layer (in the subspace of the finite dimension $(k_1, \ldots, k_n|d = \sum_{\nu=1}^{n}(k_\nu))$) and the eigenvalues are found in the form of algebraic expressions in terms of the quantum numbers $k_1, \ldots, k_n$ from Eqs. (21). Note that the algorithm for the calculation of the spectrum in the quantum problem takes more computational resources, since it assumes the calculation of the coefficients $b_{k_1,\ldots,k_n}$ in a layer of a higher dimension $(k_1, \ldots, k_n)$ (see [6]).

If $G^{(l)}$ is given in the nondiagonal representation $G^{(l)} = \sum_{k'_1,\ldots,k'_n} f_{k'_1,\ldots,k'_n}|k'_1, \ldots, k'_n\rangle$, then corrections to the eigenvalues and eigenfunctions are found from the secular equations (in a subspace of the finite dimension $(k_1, \ldots, k_n|d = \sum_{\nu=1}^{n} k_\nu)$ that is determined by approximate integrals of motion [16]). In certain cases, $G^{(l)}$ can be diagonalized by passing to new production and annihilation operators [4]; in other cases, $G^{(l)}$ are determined by solving the corresponding three-term recurrences [17].

The algorithms considered in this paper provide an efficient solution of the direct and inverse normalization problems for the class of polynomial Hamiltonians [18]; moreover, they provide means for the investigation of the dynamics of systems of coupled oscillators with polynomial interaction and atomic systems in external electromagnetic fields [19, 20].

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[3] Note that only even values of k_1 and k_2 have a physical meaning.

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