Generalisation of the explicit expression for the Deprit generator to Hamiltonians nonlinearly dependent on small parameter.

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Abstract This work explores a structure of the Deprit perturbation series and its connection to a Kato resolvent expansion. It extends the formalism previously developed for the Hamiltonians linearly dependent on perturbation parameter to a nonlinear case.

We construct a canonical intertwining of perturbed and unperturbed averaging operators. This leads to an explicit expression for the generator of the Lie-Deprit transform in any perturbation order. Using this expression, we discuss a regular pattern in the series, non-uniqueness of the generator and normalised Hamiltonian, and the uniqueness of the Gustavson integrals.

Comparison of the corresponding computational algorithm with classical perturbation methods demonstrates its competitiveness for Hamiltonians with a limited number of perturbation terms.

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Keywords Classical perturbation theory; Lie-Deprit transform; Liouvillian; Resolvent; Kato expansion

1 Introduction

In a previous article (Nikolaev 2015), we demonstrated a connection between the canonical perturbation series in classical mechanics and a Kato expansion for the resolvent of the Liouville operator. However, only the perturbations having the particular form $H_0 + \varepsilon H_1$ were considered.

In this paper we extend the formalism to general perturbed Hamiltonians represented by the power series $H = H_0 + \sum_{k=0}^{\infty} \varepsilon^k H_k$. 
Our method was inspired by the remarkable analogies between mathematical formalisms of perturbation expansions in classical and quantum mechanics. It uses Kato series for the Laurent coefficients of the resolvent of the Liouville operator (Kato 1966). The approach reveals a regular structure in the perturbation series and leads to an explicit expression for the generator of a normalising transform in any perturbation order:

$$ W = \hat{S}_H \frac{\partial H}{\partial \varepsilon}. $$

Here, $\hat{S}_H$ is the partial pseudo-inverse of the perturbed Liouville operator. The canonical intertwining of perturbed and unperturbed averaging operators allows for a description of non-uniqueness of the generator and normalised Hamiltonian. Surprisingly, Gustavson integrals are unique.

After a description of the explicit computational algorithm, we will compare its results and efficiency with those of the major canonical perturbation approaches by Gustavson (1966), Hori-Mersman (1970), Deprit (1969), Henrard (1973), and Dragt and Finn (1976). Our experiments with high-order computations for simple models demonstrate the competitiveness of the explicit algorithm for Hamiltonians with a limited number of perturbation terms.

Note that all calculations are formal, in the sense that neither a discussion of power series convergence nor conditions for the existence of constructed operators are present.

The downloadable supplementary data files (Demo 2016) contain demonstrations and large formulae. The demonstrations use the freeware computer algebra system FORM (Kuipers et al 2013).

2 Basic perturbation operators

We consider a Hamiltonian $H$ that differs from an exactly solvable one by a power series perturbation:

$$ H = H_0 + V(\varepsilon), \quad V = \sum_{k=1}^{\infty} \varepsilon^k H_k. $$

Here $H_0$ and $H_k$ are the functions of canonical variables $x = (p, q)$ on $\mathbb{R}^{2d}$ phase space:

$$ x_i = q_i, \quad x_{i+d} = p_i, \quad i = 1, \ldots, d, $$

equipped with the canonical structure (Poisson brackets):

$$ [F(x), G(x)] = \sum_{i=1}^{d} \frac{\partial F}{\partial q_i} \frac{\partial G}{\partial p_i} - \frac{\partial F}{\partial p_i} \frac{\partial G}{\partial q_i}. $$

We will discuss autonomous (time-independent) Hamiltonians having compact energy surfaces $H(p, q) = E$. We will also assume that all functions are analytic.
The goal of the canonical perturbation theory is to transform the perturbed Hamiltonian into a simpler operator using a near-identity canonical (i.e. preserving the Poisson brackets) transform:

\[ x = \mathcal{U}(\varepsilon) \tilde{x}, \quad \mathcal{U}([F, G]) = [\mathcal{U}F, \mathcal{U}G]. \]

The families of such transforms may be handled conveniently using an operator formalism (Deprit 1969; Giorgilli 2012). We will outline some of the basics of it.

**Liouvillian:** For any analytic \( W(x) \), one may introduce a Liouville operator acting in the space of analytic functions:

\[ \hat{L}_W = [\ , , W], \quad \hat{L}_W F = [F, W]. \]

Due to the Jacobi identity, the Liouvillian is the derivation of a Poisson bracket:

\[ \hat{L}_W [F, G] = [\hat{L}_W F, G] + [F, \hat{L}_W G]. \quad (1) \]

**Averaging operator:** We assume that the unperturbed Hamiltonian system with the compact energy surface \( H_0(x) = E \) is completely integrable in a Liouville sense and performs quasi-periodic motion on the invariant tori (Arnold 1978). The time average

\[ \langle F \rangle = \lim_{T \to \infty} \frac{1}{T} \int_0^T F(p(t), q(t))|_{\text{period}} \, dt = \lim_{T \to \infty} \frac{1}{T} \int_0^T e^{\hat{L}_{H_0} t} F(x) \, dt \quad (2) \]

exists in an action-angle representation for any analytic function \( F(x) \). This average is a function of the initial point \( x \). Because it is written in an invariant form, it also exists in other canonical variables.

The time averaging operation extracts from \( F(x) \) its secular non-oscillating part, which remains constant under the time evolution. In functional analysis, it is known as Cesàro \((C, 1)\) average.

However, we will use a stronger Abel average which is common in quantum physics:

\[ \langle F \rangle^{(A)} = \lim_{\lambda \to +0} \lambda \int_0^{+\infty} e^{-\lambda t} e^{\hat{L}_{H_0} t} F(x) \, dt. \]

Whenever the Cesàro average \((2)\) exists, the Abel averaging produces the same results (Hille and Phillips 1957). The Abel average greatly simplifies the formulae and leads to a natural connection to resolvent formalism. Strictly speaking, we should discuss corresponding Tauberian theorems, but we have limited our focus to formal expressions only.

The corresponding averaging operator:

\[ \hat{P}_{H_0} = \lim_{\lambda \to +0} \lambda \int_0^{+\infty} dt e^{-\lambda t} e^{\hat{L}_{H_0}}, \quad (3) \]

is a projector \( \hat{P}_{H_0}^2 = \hat{P}_{H_0} \). It projects \( F(x) \) onto the space of functions commuting with \( H_0 \). This is the kernel of \( \hat{L}_{H_0} \) and the algebra of unperturbed integrals of motion.
The notation $\hat{P}_{H_0}$ was borrowed from quantum mechanics. Other common notations for this operator are $\langle \rangle$, $\hat{F}$ and $M_t$.

Classical perturbation theory provides several recipes to compute the averaging operator. In the action-angle coordinates, the unperturbed Hamiltonian is the function of $d$ action variables $J$, and the perturbation is $2\pi$ periodic in the phases $\phi$:

$$H = H_0(J) + V(J, \phi, \varepsilon) = H_0(J) + \sum_k \tilde{V}(J, k, \varepsilon) e^{i(k, \phi)}.$$ 

The motion of the unperturbed system is quasi-periodic: $J = \text{const}$, $\phi(t) = \omega t + \phi_0$ and $\omega = \partial H_0/\partial J$. Since the Fourier components in the action-angle representation are eigenfunctions of $\hat{L}_{H_0}$, the result of the averaging operation can be written in the well-known form:

$$\hat{P}_{H_0} F = \lim_{\lambda \to +0} \lambda \int_{0}^{+\infty} e^{-\lambda t} \sum_k \tilde{\hat{F}}(J, k) e^{i(k, \phi)} e^{i(\omega k)t} dt = \sum_{(\omega, k) \neq 0} \tilde{\hat{F}}(J, k) e^{i(k, \phi)}.$$  

(4)

An another example is the Birkhoff-Gustavson representation for power series Hamiltonians (Gustavson 1966). In the simplest case, a quadratic unperturbed Hamiltonian is diagonalisable into $H_0 = \sum \omega_k (p_k^2 + q_k^2)/2$.

After the canonical transform to complex variables:

$$q_k = 1/\sqrt{2} (\xi_k + i \eta_k), \quad p_k = i/\sqrt{2} (\xi_k - i \eta_k), \quad k = 1, \ldots, d,$$

the Hamiltonian becomes:

$$H = \sum_{k=1}^{d} i \omega_k \xi_k \eta_k + \sum_{|m|+|n| \geq 3} \tilde{V}(m, n, \varepsilon) \prod_{k=1}^{d} \xi_k^m \eta_k^n.$$ 

The monomials $\xi^m \eta^n = \prod \xi_k^m \eta_k^n$ are eigenfunctions of the unperturbed Liouvillian:

$$\hat{L}_{H_0} \xi^m \eta^n = i (\omega, m - n) \xi^m \eta^n.$$ 

Therefore, for any series $F(p, q) = \sum \tilde{F}(m, n) \xi^m \eta^n$, its formal average can be computed as:

$$\hat{P}_{H_0} F = \sum_{(\omega, m - n) \neq 0} \tilde{\hat{F}}(m, n) \xi^m \eta^n.$$ 

Integrating operator: The complementary projector $1 - \hat{P}_{H_0}$ extracts the time-oscillating part from $F(x)$. It projects on the non-secular space of oscillating functions where the inverse of $\hat{L}_{H_0}$ exists (we will consider only the semi-simple $\hat{L}_{H_0}$).

This inverse is called the integrating operator $\hat{S}_{H_0}$; it is also called the solution of the homological equation, tilde operation, zero-mean antiderivative, Friedrichs $\hat{I}$ operation, $1/k$ operator and division operation. Its invariant definition was given by Primas (1963):

$$\hat{S}_{H_0} = - \lim_{\lambda \to +0} \lambda \int_{0}^{+\infty} dt e^{-\lambda t} e^{\hat{L}_{H_0}} (1 - \hat{P}_{H_0}).$$  

(5)
In the action-angle representation, the result of the integrating operator is as follows:

\[ \mathbf{S}_{H_0} F = \sum_{(\alpha, k \neq 0)} \frac{1}{i(\alpha, k)} \hat{F}(\mathbf{J}, k) e^{i(k, \phi_0)}. \]  

(6)

According to KAM theory (Kolmogorov 1953), for a general nondegenerate multidimensional system, the operator (6) is analytic for almost all frequencies except a set of Lebesgue measure zero. This suffices for our formal constructions.

The corresponding expression in the Birkhoff-Gustavson representation is:

\[ \mathbf{S}_{H_0} F = \sum_{(\alpha, m - n \neq 0)} \frac{1}{i(\alpha, m - n)} \hat{F}(m, n) \zeta^m \eta^n. \]

The operators \( \mathbf{L}_{H_0}, \mathbf{P}_{H_0} \) and \( \mathbf{S}_{H_0} \) are the building blocks of the canonical perturbation series presented here. It is easy to check that:

\[ \mathbf{L}_{H_0} \mathbf{S}_{H_0} = \mathbf{S}_{H_0} \mathbf{L}_{H_0} = 1 - \mathbf{P}_{H_0}, \]

\[ \mathbf{S}_{H_0} \mathbf{P}_{H_0} = \mathbf{P}_{H_0} \mathbf{S}_{H_0} \equiv 0. \]

Further canonical identities have been discussed in Nikolaev (2015).

3 Canonical perturbation theory

It is known (Arnold 1978) that any near-identity family of canonical transforms

\[ x = \hat{U}(\epsilon) \mathbf{x}, \quad \hat{H} = \hat{U} H, \]

is a Hamiltonian flow in time \( \epsilon \) with some generator \( W(x, \epsilon) \). The corresponding operators obey the equations:

\[ \frac{\partial \hat{U}}{\partial \epsilon} = \hat{U} \hat{L}, \quad \frac{\partial \hat{U}^{-1}}{\partial \epsilon} = -\hat{L} \hat{U}^{-1}. \]  

(7)

In classical mechanics, such \( \epsilon \)-dependent parameterisations are called Lie-Deprit transforms (Deprit 1969). In quantum physics, corresponding objects are known as ordered exponentials (Dyson 1949).

When comparing the quantum analogues (Suzuki 1985; Nikolaev 2016), we should mention that the classical Lie-Deprit transform \( \hat{U}_W \) corresponds to the negative ordered quantum exponential \( \exp(-\int L_{-W} ds) \), the inverse transform \( \hat{U}_W^{-1} \) corresponds to the positive ordered exponential \( \exp(\int L_{-W} ds) \) and the generator has the opposite sign.

The perturbation theory constructs the transforms and the generator in the form of a power series:

\[ \hat{U}_W = \sum_{n=0}^{\infty} \epsilon^n \hat{U}_n, \quad \hat{U}_W^{-1} = \sum_{n=0}^{\infty} \epsilon^n \hat{U}_n^{-1}, \quad W(x, \epsilon) = \sum_{n=0}^{\infty} \epsilon^n W_n(x). \]
To demonstrate the regular structure of the perturbative series, we do not include factorial denominators in the above expressions, which is traditionally done. To avoid any misunderstandings, we should note that $\hat{U}_n^{-1}$ means the operator coefficient of $\varepsilon^n$ in the series for $\hat{U}_n^{-1}$. This is not the inverse of the $\hat{U}_n$ coefficient.

The substitution of the series for $W$, $\hat{U}$ and $\hat{U}^{-1}$ into the equations (7) results in the following recursive relations for the coefficients:

$$
\hat{U}_n = -\frac{1}{n} \sum_{k=0}^{n-1} \hat{U}_k \hat{L}_{W_{n-k}}, \quad \hat{U}_n^{-1} = -\frac{1}{n} \sum_{k=0}^{n-1} \hat{L}_{W_{n-k}} \hat{U}_k^{-1}.
$$

(8)

Iterating these expressions, Cary (1981) obtained the non-recursive formulae:

$$
0_n = \sum_{(m_1, \ldots, m_r) \in \mathbb{N}} \frac{L_{W_{m_r-1}}}{m_r} \cdots \frac{L_{W_{m_1-1}}}{m_1} \frac{L_{W_{m_1-1}}}{n},
$$

$$
0_n^{-1} = \sum_{(m_1, \ldots, m_r) \in \mathbb{N}} (-1)^{r+1} \frac{L_{W_{m_1-1}}}{n} \cdots \frac{L_{W_{m_r-1}}}{m_r}.
$$

The sum runs over all sets of integers $(m_1, \ldots, m_r)$, satisfying $n > m_1 > \cdots > m_r > 0$.

In this paper, we will derive a similar formula for the normalising generator.

The canonical perturbation theory constructs $W = \sum_0^\infty \varepsilon^n W_n(x)$ to simplify the transformed Hamiltonian as much as possible. In the first order:

$$
\tilde{H} = \hat{U}_0(H_0 + \sum_{k=0}^{\infty} \varepsilon^k H_k) = H_0 + \varepsilon(H_1 + \hat{L}_{W_0}H_0) + O(\varepsilon^2)
$$

$$
= H_0 + \varepsilon \left( H_1 - \hat{L}_{W_0}W_0 \right) + O(\varepsilon^2).
$$

If one choose $W_0 = \tilde{S}_{H_0}H_1$ in the above expression, then all the terms of order $\varepsilon$ in the transformed Hamiltonian become secular (beginning with $\hat{P}_{H_0}$ operator):

$$
\tilde{H} = H_0 + \varepsilon \hat{P}_{H_0}H_1 + O(\varepsilon^2).
$$

Typically, a perturbation method constructs the normalising generator and the transformed Hamiltonian order by order. It consequentially chooses $W_1$ to eliminate non-secular terms up to $\varepsilon^2$, then $W_2$ to eliminate nonsecular terms up to $\varepsilon^3$, and so on. The detailed description of such procedures can be found in classical books on the perturbation theory (Nayfeh 1973; Giacaglia 1972; Ferraz-Mello 2007).

Obviously, the generator $W$ is not unique. An arbitrary secular function $\hat{P}_{H_0}F$ may be added to any order. Further orders will depend on this term. The rule for choosing the secular part of $W$ is the uniqueness condition. It is common to construct a completely non-secular generator $\hat{P}_{H_0}W_{NS} = 0$. However, we will see that other conditions may be useful.

If the process converges, the canonical transform with the generator $W = \sum_0^\infty \varepsilon^n W_n$ makes the Hamiltonian completely secular:

$$
\hat{P}_{H_0}\tilde{H} = \tilde{H}.
$$
or equivalently, \( \hat{U}_W^{-1} \hat{P}_H \hat{U}_W \hat{H} = H \).

Conversely, if we construct an analytic continuation of the averaging operator \( \hat{P}_{H_0} \) to the perturbed case

\[
\hat{P}_H(\epsilon) H(\epsilon) = H, \quad \hat{P}_H(0) = \hat{P}_{H_0},
\]

and a transform, such that the perturbed and unperturbed projectors are canonically connected

\[
\hat{P}_H = \hat{U}_W^{-1} \hat{P}_{H_0} \hat{U}_W,
\]

then, due to the intertwining properties of this transform

\[
\hat{U}_W \hat{P}_H = \hat{P}_{H_0} \hat{U}_W, \quad \hat{P}_H \hat{U}_W^{-1} = \hat{U}_W^{-1} \hat{P}_{H_0},
\]

a new Hamiltonian will become secular:

\[
\hat{P}_{H_0} \tilde{H} = \hat{P}_{H_0} \hat{U}_W \hat{H} = \hat{U}_W \hat{P}_H \hat{H} = \hat{U}_W H = \tilde{H}.
\]

Therefore, this construction will explicitly realise the goal of the canonical perturbation theory. In the next sections, we will develop such a continuation and intertwining canonical transform using the methods of functional analysis.

### 4 The Liouvillian resolvent

Consider the resolvent of the Liouville operator:

\[
\hat{R}_H(z) = (\hat{L}_H - z)^{-1}.
\]

This operator-valued function of the complex variable \( z \) is the Laplace transform of the evolution operator of the Hamiltonian system:

\[
\hat{R}_H(z) = -\int_0^{+\infty} dt \, e^{-zt} \hat{e}^{\hat{L}H}.
\]

Resolvent singularities are the eigenvalues of \( \hat{L}_H \). For an integrable Hamiltonian system with compact energy surfaces, these eigenvalues belong to an imaginary axis. Typically, the spectrum of a Liouville operator is anywhere dense (Spohn 1975).

Let us begin with a simple case of an isolated point spectrum. We consider a one-dimensional system and restrict the domain of the resolvent operator to analytic functions with the argument on the compact energy surface \( H(x) = E \). Under such conditions, the system is non-relaxing and oscillates with the single frequency \( \omega(E) \).

The resolvent singularities are located at the points \( 0, \pm i\omega(E), \pm 2i\omega(E), \ldots \).

The existence of the operator \( \hat{P}_{H_0} \) defined by (3) means that the unperturbed resolvent has a simple pole at 0. The averaging operator is the residue of the resolvent at that pole:

\[
\hat{P}_{H_0} \equiv -\text{Res}_{z=0} \hat{R}_{H_0},
\]

while the integrating operator \( \hat{S}_{H_0} \) is its holomorphic part:

\[
\hat{S}_{H_0} = \lim_{z \to 0} \hat{R}_{H_0}(z) \left( 1 - \hat{P}_{H_0} \right).
\]
Therefore, the Liouvillian resolvent combines both of the basic perturbation operators (Nikolaev 2015). This allows us to apply the powerful formalism of complex analysis to the perturbation theory.

It is well known (Kato 1966) that, due to the Hilbert resolvent identity:

$$\hat{\mathcal{R}}_H(z_1) - \hat{\mathcal{R}}_H(z_2) = (z_1 - z_2) \hat{\mathcal{R}}_H(z_1) \hat{\mathcal{R}}_H(z_2),$$

(12)

the Laurent series for the unperturbed resolvent has the form of a geometric progression:

$$\hat{\mathcal{R}}_H^0(z) = -\frac{1}{z} \hat{\mathcal{P}}_H + \sum_{n=0}^{\infty} z^n \hat{\mathcal{S}}_H^n = \sum_{n=0}^{+\infty} \hat{\mathcal{R}}^{(n)}_H z^{n-1}.$$  

(13)

Here, we denoted $\hat{\mathcal{R}}^{(0)}_H = -\hat{\mathcal{P}}_H$ and $\hat{\mathcal{R}}^{(n)}_H = \hat{\mathcal{S}}_H^n$.

The perturbed resolvent may be more singular. The Laurent series for a general resolvent with an isolated singularity at the origin has the following form (Kato 1966):

$$\hat{\mathcal{R}}_H(z) = -\frac{1}{z} \hat{\mathcal{P}}_H + \sum_{n=0}^{\infty} z^n \hat{\mathcal{S}}_H^n - \sum_{n=2}^{\infty} z^{-n} \hat{\mathcal{D}}_H^n = \sum_{n=-\infty}^{+\infty} \hat{\mathcal{R}}^{(n)}_H z^{n-1},$$

where $\hat{\mathcal{D}}_H$ is the eigen-nilpotent operator, which does not have an unperturbed analogue ($\hat{\mathcal{D}}_H^0 \equiv 0$).

4.1 Kato series

In our case of the isolated point spectrum, the perturbed resolvent can be expanded into the Neumann series. Since

$$\hat{L}_{H_0 + V} - z = \left(1 + \hat{L}_V \hat{\mathcal{R}}_H(z) \right) \left(\hat{L}_H - z\right),$$

then for $V = \sum_{k=1}^{\infty} \epsilon^k H_k$, the following expansion holds:

$$\hat{\mathcal{R}}_H(z) = \hat{\mathcal{R}}_H(1 + \hat{L}_V \hat{\mathcal{R}}_H(z))^{-1} = \hat{\mathcal{R}}_H(z) \sum_{n=0}^{\infty} (-\hat{L}_V \hat{\mathcal{R}}_H(z))^n = \hat{\mathcal{R}}_H(z) + \sum_{n=1}^{\infty} \epsilon^n \hat{\mathcal{R}}^{(n)}_H(z).$$

(14)

The coefficient operators are given by the expression:

$$\hat{\mathcal{R}}^{(n)}_H(z) = \sum_{m=1}^{n} (-1)^m \sum_{k_1 + \cdots + k_m = n \atop k_j \geq 0} \hat{\mathcal{R}}_H(z) \hat{L}_{H_{k_1}} \hat{\mathcal{R}}_H(z) \cdots \hat{L}_{H_{k_m}} \hat{\mathcal{R}}_H(z),$$

where the sum being taken for all combinations of $1 \leq m \leq n$ positive integers $k_1, \ldots, k_m$, such that $k_1 + \cdots + k_m = n$.

The integration around a sufficiently small contour $|z| = a$ encompassing the singularity at the origin results in the Kato series for the perturbed averaging operator (Kato 1966):

$$\hat{\mathcal{P}}_H = -\frac{1}{2\pi i} \oint_{|z|=a} \hat{\mathcal{R}}_H(z) dz$$
\[ \hat{P}_H = \frac{1}{2\pi i} \sum_{n=1}^{\infty} \frac{1}{e^n} \int_{|z|=\epsilon} \sum_{m=0}^{n} (-1)^m \sum_{k_1+\ldots+k_m=n} \hat{\mathcal{L}}_{H_0}(z) \hat{L}_{H_0}(z) \ldots \hat{L}_{H_0}(z) \hat{\mathcal{L}}_{H_0}(z) \, dz \]

\[ = \hat{P}_H - \frac{1}{2\pi i} \sum_{n=1}^{\infty} e^n \int_{|z|=\epsilon} \sum_{m=0}^{n} (-1)^m \sum_{k_1+\ldots+k_m=n} \left( \sum_{p_{n+1}=0}^{\infty} \hat{\mathcal{L}}_{H_0}^{(p_{n+1})} \hat{L}_{H_0}^{(p_0)} \right) \hat{\mathcal{L}}_{H_0}(z) \hat{L}_{H_0}(z) \ldots \hat{L}_{H_0}(z) \hat{\mathcal{L}}_{H_0}(z) \, dz. \]

The perturbed integrating operator and the perturbed eigen-nilpotent operator are:

\[ \hat{S}_H = \frac{1}{2\pi i} \int_{|z|=\epsilon} z^{-1} \hat{\mathcal{L}}_{H}(z) \, dz, \quad \hat{D}_H = -\frac{1}{2\pi i} \int_{|z|=\epsilon} z \hat{\mathcal{L}}_{H}(z) \, dz. \]

Only the coefficients of $z^{-1}$ in the above expressions will contribute to the result:

\[ \hat{P}_H = \hat{P}_H + \sum_{n=1}^{\infty} e^n \left( \sum_{m=0}^{n} (-1)^m \sum_{p_1+\ldots+p_{n+1}=m} \hat{\mathcal{L}}_{H_0}^{(p_{n+1})} \hat{L}_{H_0}^{(p_0)} \hat{\mathcal{L}}_{H_0}(z) \hat{L}_{H_0}(z) \ldots \hat{L}_{H_0}(z) \hat{\mathcal{L}}_{H_0}(z) \right). \]

\[ \hat{S}_H = \hat{S}_H + \sum_{n=1}^{\infty} e^n \left( \sum_{m=0}^{n} (-1)^m \sum_{p_1+\ldots+p_{n+1}=m+1} \hat{\mathcal{L}}_{H_0}^{(p_{n+1})} \hat{L}_{H_0}^{(p_0)} \hat{\mathcal{L}}_{H_0}(z) \hat{L}_{H_0}(z) \ldots \hat{L}_{H_0}(z) \hat{\mathcal{L}}_{H_0}(z) \right). \]

\[ \hat{D}_H = \sum_{n=1}^{\infty} e^n \left( \sum_{m=0}^{n} (-1)^m \sum_{p_1+\ldots+p_{n+1}=m+1} \hat{\mathcal{L}}_{H_0}^{(p_{n+1})} \hat{L}_{H_0}^{(p_0)} \hat{\mathcal{L}}_{H_0}(z) \hat{L}_{H_0}(z) \ldots \hat{L}_{H_0}(z) \hat{\mathcal{L}}_{H_0}(z) \right). \]

(15)

Because the operator $\hat{\mathcal{L}}_{H_0}^{(p_0)}$ consists of $p_j$ operators $\hat{S}_H$, the summation in the coefficient of $e^n$ in the above expressions is being taken by all possible subdivisions of $n$ in $m$ parts by perturbations $\hat{L}_{H_0}$ and all placements of $m$ (or $m+1$, or $m-1$) integrating operators $\hat{S}_H$ in these parts. For example, the first two orders of the perturbed integrating operator are:

\[ \hat{S}_H = \hat{S} + e \left( \hat{S}_H^2 \hat{\mathcal{L}}_{H} \hat{P} + \hat{\mathcal{L}}_{H} \hat{S}_H^2 - \hat{S}_H \hat{\mathcal{L}}_{H} \hat{S} + \hat{\mathcal{L}}_{H} \hat{S} \hat{S}_H^2 + \hat{\mathcal{L}}_{H} \hat{S}_H \hat{\mathcal{L}}_{H} \hat{S} - \hat{S}_H \hat{\mathcal{L}}_{H} \hat{S}_H \hat{\mathcal{L}}_{H} \hat{S} \right) + O(e^3). \]
Here we omitted the subscript $H_0$ for the unperturbed $\hat{P}_{H_0}$ and $\hat{S}_{H_0}$ operators.

The properties of the unperturbed operators can be extended to their analytic continuations as follows:

\[
\begin{align*}
\hat{P}_H H &= H, & \hat{S}_H L_H &= L_H \hat{S}_H = 1 - \hat{P}_H, & \hat{L}_H \hat{P}_H &= \hat{P}_H \hat{L}_H = \hat{D}_H, \\
\hat{S}_H \hat{P}_H &= 0, & \hat{P}_H \hat{D}_H &= \hat{D}_H \hat{P}_H = \hat{D}_H.
\end{align*}
\]  

(16)

For the details, refer to Nikolaev (2015).

To avoid any misunderstandings, it should be noted that $\hat{P}_H F$ will not be commuting with the perturbed Hamiltonian. This is because, in general, $L_H \hat{P}_H = \hat{D}_H \neq 0$. Actually, the perturbed projector, $\hat{P}_H$, projects onto some analytic continuation of the algebra of the integrals of the unperturbed Hamiltonian. This may not coincide with the algebra of the integrals of the perturbed system because of a destruction of symmetries.

### 4.2 Canonical properties of the Liouvillian resolvent

Since $\hat{L}$ is a derivative, there exists an integration by parts formula for its resolvent. It results from the application of the identical operator

\[
\hat{R}_H(z_1) \left( L_H - z_1 \right) \equiv 1,
\]

to the Poisson bracket $\hat{L} \hat{R}_{H(z_2)} F \hat{R}_H(z_3)$. We suppose that complex $z_1$, $z_2$, and $z_3$ are outside of the spectrum of $L_H$ and that an arbitrary function $F(x)$ is analytic.

An expansion of the Jacobi identity $L_F \hat{L}_G - \hat{L}_G L_F = L_{LFG}$ yields:

\[
\begin{align*}
\hat{L}_{\hat{R}_{H(z_2)} F} \hat{R}_H(z_3) &= \hat{R}_H(z_1) \hat{L}_H \hat{L}_{\hat{R}_{H(z_2)} F} \hat{R}_H(z_3) - z_1 \hat{R}_H(z_1) \hat{L}_{\hat{R}_{H(z_2)} F} \hat{R}_H(z_3) \\
&= \hat{R}_H(z_1) \hat{L}_{\hat{R}_{H(z_2)} F} \hat{L}_H \hat{R}_H(z_3) + \hat{R}_H(z_1) \hat{L}_{\hat{R}_{H(z_2)} F} \hat{R}_H(z_3) \\
&\quad - z_1 \hat{R}_H(z_1) \hat{L}_{\hat{R}_{H(z_2)} F} \hat{R}_H(z_3) \\
&= \hat{R}_H(z_1) \hat{L}_{\hat{R}_{H(z_2)} F} \left( 1 + z_3 \hat{R}_H(z_3) \right) + \hat{R}_H(z_1) \hat{L}_{1 + z_3 \hat{R}_{H(z_2)} F} \hat{R}_H(z_3) \\
&\quad - z_1 \hat{R}_H(z_1) \hat{L}_{\hat{R}_{H(z_2)} F} \hat{R}_H(z_3).
\end{align*}
\]

Therefore, the following identity holds true for the Liouvillian resolvent:

\[
\hat{R}_H(z_1) \hat{L}_F \hat{R}_H(z_3) = \hat{L}_{\hat{R}_{H(z_2)} F} \hat{R}_H(z_3) - \hat{R}_H(z_1) \hat{L}_{\hat{R}_{H(z_2)} F} + (z_1 - z_3) \hat{R}_H(z_1) \hat{L}_{\hat{R}_{H(z_2)} F} \hat{R}_H(z_3).
\]  

(17)

Consider the derivative of the resolvent with respect to the perturbation

\[
\frac{\partial}{\partial \epsilon} \left( \hat{R}_H(z) \right) = -\hat{R}_H(z) \hat{L}_{\partial H/\partial \epsilon} \hat{R}_H(z).
\]
Substituting $z_1 = z_2 = z$ and $\mathcal{F} = \partial H / \partial \varepsilon$ in the canonical identity (17) yields:

$$\hat{R}_H(z) L_{\partial H / \partial \varepsilon} \hat{R}_H(z) = \hat{L}_{R_t(z)} \hat{R}_H(z) - \hat{R}_H(z) \hat{L}_{R_t(z)} \partial H / \partial \varepsilon$$

$$- z \hat{R}_H(z) \hat{L}_{R_t(z)} \partial H / \partial \varepsilon \hat{R}_H(z).$$

Finally, we obtain the following series:

$$\frac{\partial}{\partial \varepsilon} \hat{R}_H(z) = \hat{R}_H(z) \hat{L}_{\partial_0 H / \partial \varepsilon} - \hat{L}_{\partial_0 H / \partial \varepsilon} \hat{R}_H(z) - \hat{R}_H(z) \hat{L}_{\partial_0 H / \partial \varepsilon} \hat{R}_H(z).$$

Proceeding in a similar way for the coefficients of $z^{-n}$ ($n \geq 1$) in (18), we obtain:

$$\hat{R}_H(z) \hat{L}_{\partial_0 H / \partial \varepsilon} = \hat{L}_{\partial_0 H / \partial \varepsilon} \hat{R}_H(z) - \hat{R}_H(z) \hat{L}_{\partial_0 H / \partial \varepsilon} \hat{R}_H(z),$$

$$\hat{R}_H(z) \hat{L}_{\partial_0 H / \partial \varepsilon} = \hat{L}_{\partial_0 H / \partial \varepsilon} \hat{R}_H(z) - \hat{R}_H(z) \hat{L}_{\partial_0 H / \partial \varepsilon} \hat{R}_H(z).$$

This allows us to rewrite the expression for the resolvent derivative as:

$$\frac{\partial}{\partial \varepsilon} \hat{R}_H(z) = \hat{R}_H(z) \hat{L}_{\partial_0 H / \partial \varepsilon} - \hat{L}_{\partial_0 H / \partial \varepsilon} \hat{R}_H(z) - \hat{R}_H(z) \hat{L}_{\partial_0 H / \partial \varepsilon} \hat{R}_H(z) + \ldots$$

Actually, this is a power series because $\hat{R}_H^o = O(\varepsilon^0)$.

It follows from the Hilbert resolvent identity that:

$$\hat{H}_H = O(\varepsilon^0).$$

Finally, we obtain the following series:

$$\frac{\partial}{\partial \varepsilon} \hat{R}_H(z) = \hat{R}_H(z) \hat{L}_{\partial_0 H / \partial \varepsilon} - \hat{L}_{\partial_0 H / \partial \varepsilon} \hat{R}_H(z) - \hat{R}_H(z) \hat{L}_{\partial_0 H / \partial \varepsilon} \hat{R}_H(z) + \hat{R}_H(z) \hat{L}_{\partial_0 H / \partial \varepsilon} \hat{R}_H(z) + \ldots$$

The derivative of the projector $\partial \hat{P}_H / \partial \varepsilon$ can be obtained as the residue of this expression at $z = 0$. In the case of an isolated point spectrum, the Liouvillian resolvent is a meromorphic function and, therefore the residue of any of its derivatives with respect to $z$ vanishes identically. As a result, the projector $\hat{P}_H$ transforms canonically under the perturbation:

$$\frac{\partial}{\partial \varepsilon} \hat{P}_H = \hat{P}_H \hat{L}_{\partial_0 H / \partial \varepsilon} - \hat{L}_{\partial_0 H / \partial \varepsilon} \hat{P}_H,$$

and the projectors are connected by the canonical Lie-Deprit transform:

$$\hat{P}_H = \hat{U}_H \hat{P}_0 \hat{U}_H^*, \quad W = \hat{S}_H \partial H / \partial \varepsilon.$$

This holds for all perturbation orders.
5 An explicit expression for a generator

5.1 Regular pattern in perturbation series

As was discussed, the canonical connection of the projectors means that the Lie-Deprit transform with the generator

\[ W = \hat{S}_H \frac{\partial H}{\partial \varepsilon} \]  (21)

formally normalises the Hamiltonian in all orders in \( \varepsilon \). The expanded form of this expression demonstrates the regular pattern:

\[ W = \sum_{n=0}^{\infty} \varepsilon^n \left( \sum_{m=0}^{n} (-1)^m \sum_{p_0+\cdots+p_m=m+1 \atop k_0+\cdots+k_m=m+1} k_0 \hat{R}^{(p_0)}_{H_0} \hat{L}_{H_{p_0}} \hat{R}^{(p_1)}_{H_0} \cdots \hat{R}^{(p_m)}_{H_0} \hat{L}_{H_{k_0}} \right) \]  (22)

Here, the sum being taken for all the combinations of positive integers \( k_0, \ldots, k_m \) and nonnegative \( p_0, \ldots, p_m, 1 \leq m \leq n \) such that \( \sum p_j = m + 1 \), and \( \sum k_j = n + 1 \). The first two perturbative orders for the generator are:

\[ W = \hat{S}H_1 + \varepsilon \left( \hat{S}^2 \hat{L}_{H_1} \hat{P}H_1 - \hat{S} \hat{L}_{H_1} \hat{S}H_1 + 2 \hat{S}H_2 \right) + \varepsilon^2 \left( \hat{S}L_{H_1} \hat{S}L_{H_1} \hat{S}H_1 - \hat{S}L_{H_1} \hat{P}L_{H_1} \hat{S}H_1 - \hat{S}L_{H_1} \hat{S}L_{H_1} \hat{S}^2 H_1 \right. \]

\[ + \hat{S}P_{H_1} \hat{S}^2 \hat{L}_{H_1} \hat{S}H_1 + \hat{P}L_{H_1} \hat{S}^2 \hat{L}_{H_1} \hat{S}H_1 + \hat{P}L_{H_1} \hat{P}L_{H_1} \hat{S}^3 H_1 + 3 \hat{S}H_3 - 2 \hat{S}L_{H_1} \hat{S}H_2 \]

\[ - \hat{S}L_{H_1} \hat{S}H_1 + 2 \hat{S}^2 \hat{L}_{H_1} \hat{P}H_2 + \hat{S}^2 \hat{L}_{H_1} \hat{P}H_1 + 2 \hat{P}L_{H_1} \hat{S}^2 H_2 + \hat{P}L_{H_1} \hat{S}^2 H_1 \big) + O(\varepsilon^3). \]

The four orders for the normalised Hamiltonian are:

\[ \tilde{H} = H_0 + \varepsilon \hat{P}H_1 + \varepsilon^2 \left( -\frac{1}{2} \hat{P}L_{H_1} \hat{S}H_1 + \hat{P}H_2 \right) \]

\[ + \varepsilon^3 \left( \frac{1}{3} \hat{P}L_{H_1} \hat{S}L_{H_1} \hat{S}H_1 - \frac{1}{6} \hat{P}L_{H_1} \hat{S}^2 L_{H_1} \hat{P}H_1 - \hat{P}L_{H_1} \hat{S}L_{H_1} \hat{S}H_1 \right) \]

\[ + \varepsilon^4 \left( \frac{1}{6} \hat{P}L_{H_1} \hat{S}L_{H_1} \hat{S}^2 L_{H_1} \hat{P}H_1 - \frac{1}{4} \hat{P}L_{H_1} \hat{S}^2 L_{H_1} \hat{S}H_1 + \frac{1}{12} \hat{P}L_{H_1} \hat{S}^2 L_{H_1} \hat{S}L_{H_1} \hat{P}H_1 \right) \]

\[ + \frac{1}{8} \hat{P}L_{H_1} \hat{S}L_{H_1} \hat{P}L_{H_1} \hat{S}H_1 + \frac{1}{4} \hat{P}L_{H_1} \hat{P}L_{H_1} \hat{S}^2 L_{H_1} \hat{S}H_1 + \frac{1}{4} \hat{P}L_{H_1} \hat{P}L_{H_1} \hat{S}L_{H_1} \hat{S}^2 H_1 \]

\[ - \frac{1}{6} \hat{P}L_{H_1} \hat{P}L_{H_1} \hat{S}L_{H_1} \hat{H}_1 - \frac{1}{4} \hat{P}L_{H_1} \hat{P}L_{H_1} \hat{P}L_{H_1} \hat{S}^2 H_1 + \frac{1}{2} \hat{P}L_{H_1} \hat{P}L_{H_1} \hat{S}H_2 \]

\[ + \frac{1}{4} \hat{P}L_{H_1} \hat{S}L_{H_1} \hat{S}H_1 - \frac{1}{4} \hat{P}L_{H_1} \hat{S}^2 L_{H_1} \hat{P}H_2 - \frac{1}{12} \hat{P}L_{H_1} \hat{S}^2 L_{H_1} \hat{P}H_1 - \frac{1}{2} \hat{P}L_{H_1} \hat{P}L_{H_1} \hat{S}^2 H_2 \]

\[ - \frac{1}{4} \hat{P}L_{H_1} \hat{P}L_{H_1} \hat{S}^2 H_1 + \frac{1}{4} \hat{P}L_{H_1} \hat{S}L_{H_1} \hat{P}H_1 - \frac{1}{6} \hat{P}L_{H_1} \hat{S}^2 L_{H_1} \hat{P}H_1 - \frac{1}{2} \hat{P}L_{H_1} \hat{S}H_2 \]

\[ - \hat{P}L_{H_1} \hat{S}H_1 + \hat{P}H_2 \big) + O(\varepsilon^5). \]
Here we omitted the indices $H_0$ for the unperturbed operators $\hat{P}_{H_0}$ and $\hat{S}_{H_0}$ for compactness and we took into account the identities $\hat{P}_{H_0}\hat{L}_F\hat{S}_{H_0}F \equiv 0$ and $\hat{P}_{H_0}\hat{L}_F\hat{P}_{H_0}F \equiv 0$ (Nikolaev 2015). These expressions are the generalisation of the classic result by Burshtein and Solov’ev (1961).

It is possible to extend formula (22) to multidimensional systems in the form of an asymptotic series. Similarly to previous work (Nikolaev 2015), it can be shown that the expression for $W$ truncated at order $O(\epsilon^N)$ normalises Hamiltonian up to $O(\epsilon^{N+1})$. For clarity, we here use formal analytic expressions. However, for multidimensional systems, these expressions should be converted straightforwardly into truncated sums, and all equalities hold up to $O(\epsilon^{N+1})$.

5.2 General form of the generator

Let us determine the general form of a generator of a transform connecting the perturbed and unperturbed projectors. It follows from (9) that $\hat{P}_H$ satisfies the operatorial differential equation:

$$\frac{\partial}{\partial \epsilon} \hat{P}_H = \hat{P}_H\hat{L}_W - \hat{L}_W \hat{P}_H.$$

Application of this expression to the Hamiltonian $H$ and the identities

$$\hat{P}_H H = H, \quad \frac{\partial}{\partial \epsilon} \left(\hat{P}_H H\right) = \left(\frac{\partial}{\partial \epsilon} \hat{P}_H\right) H + \hat{P}_H \frac{\partial}{\partial \epsilon} H,$$

yield

$$\left(1 - \hat{P}_H\right) \hat{L}_W = \left(1 - \hat{P}_H\right) \frac{\partial H}{\partial \epsilon}.$$

To solve this equation, it is sufficient to apply the $\hat{S}_H$ operator. Therefore, the general form of the generator of the connecting transform is:

$$W = \hat{S}_H \frac{\partial H}{\partial \epsilon} + \hat{P}_H F,$$

where $F(x, \epsilon)$ may be any analytic function, and $\hat{P}_H$ and $\hat{S}_H$ are given by (15).

This formula provides the non-recursive expression for the Deprit generator of a normalising transform and defines it unambiguously. It generalises the corresponding formula in Nikolaev (2015).

The choice of $\hat{P}_H F(x, \epsilon)$ is the uniqueness condition. It is natural to set $F \equiv 0$ or

$$\hat{P}_H W = 0.$$  

This is not equal to the non-secular condition $\hat{P}_{H_0}W_{NS} = 0$, which is traditionally used in the canonical perturbation theory. Because $\hat{L}_{\rho_{HF}}\hat{P}_H = \hat{P}_H\hat{L}_{\rho_{HF}}$, the projector $\hat{P}_H$ is itself insensitive to this choice.

We can conclude that the generators of normalising transforms can differ by a function belonging to a continuation of the algebra of the integrals of the unperturbed system.
Hamiltonians that were normalised using the different uniqueness conditions $F_1(x, \epsilon)$ and $F_2(x, \epsilon)$ are connected by a canonical transform $\hat{U}_{21} = \hat{U}_{w_1} \hat{U}_{w_1}^{-1}$. Let us find its generator:

$$\frac{\partial}{\partial \epsilon} \hat{U}_{21} = \hat{U}_{w_1} \left( \hat{L}_{w_2} - \hat{L}_{w_1} \right) \hat{U}_{w_1}^{-1} = \hat{U}_{w_2} \hat{L}_{\hat{p}_H(F_2 - F_1)} \hat{U}_{w_1}^{-1} = \hat{U}_{21} \hat{L}_{\hat{p}_H(F_2 - F_1)}.$$ 

Here, we have used the invariance of Poisson brackets by canonical transforms $\hat{L}_{\hat{p}_H} \hat{U}_{w_1} = \hat{U}_{w_1} \hat{L}_{\hat{p}_H}$. Because of the intertwining relation (10), this generator is always secular:

$$W_{21} = \hat{U}_{w_1} \hat{p}_H (F_2 - F_1) = \hat{p}_{H_0} \hat{U}_{\hat{S}_H(\partial \epsilon) + \hat{p}_H F_2} (F_2 - F_1).$$

Therefore, the secular normalised Hamiltonians obtained using different uniqueness conditions are related by the Lie-Deprit transform with the secular generator. This corresponds to the Bruno theorem for generating functions (Bruno 1989).

For the non-resonance system with incommensurable frequencies, all the integrals commute. As a consequence, a non-resonance normalised Hamiltonian is unique (Koseleff 1994).

This is not so in the case of resonance. Because resonance relations lead to non-commuting integrals, the normalised resonance Hamiltonian depends on the uniqueness condition. We can obtain an explicitly secular expression for the Hamiltonian following Vittot (1987). For the generator $W$ given by (23), consider the derivative:

$$\frac{\partial}{\partial \epsilon} \hat{H} = \left( \frac{\partial}{\partial \epsilon} \hat{U}_W \right) \hat{H} + \hat{U}_W \frac{\partial}{\partial \epsilon} \hat{H} = \hat{U}_W \left( \hat{L}_W H + \frac{\partial H}{\partial \epsilon} \right)$$

$$= \hat{U}_W \frac{\partial H}{\partial \epsilon} - \hat{L}_W \left( \hat{S}_H \frac{\partial H}{\partial \epsilon} + \hat{p}_H F \right) = \hat{U}_W \left( \hat{p}_H \frac{\partial H}{\partial \epsilon} - \hat{D}_H F \right)$$

Here, we used (7), the properties of the perturbed operators (16) and the intertwining of projectors (10). Therefore,

$$\hat{H} = H_0 + \hat{p}_{H_0} \int_0^\epsilon \hat{U}_{\hat{S}_H(\partial \epsilon) + \hat{p}_H F} \left( \frac{\partial H}{\partial \epsilon} - \hat{D}_H F \right) d\epsilon. \quad (25)$$

This secular expression demonstrates the explicit dependence on $\hat{p}_H F$. However, it requires more computational resources than the standard normalisation.

5.3 Gustavson integrals

It is interesting to find physically meaningful quantities that do not depend on an artificial choice of the uniqueness condition $\hat{p}_H F(x, \epsilon)$. Our previous work (Nikolaev 2015) demonstrated that for linearly perturbed systems, the Gustavson integrals have such a property. Now, we are able to apply similar considerations to a general case.

Consider a system with constant unperturbed frequencies that obey $r$ linearly independent resonance relations $(\omega, D_k) = 0$, $k = 1, \ldots, r$. Such resonance relations
result in additional non-commuting integrals. In the Birkhoff and action-angle representations, the centre of the corresponding algebra consist of the $d - r$ quantities:

$$I_m = \sum_{j=1}^{d} \beta_m \xi_j \bar{\eta}_j = (\beta_m, J), \quad m = 1, \ldots, d - r,$$

where $\bar{\beta}_m$ is a set of $d - r$ independent vectors that are orthogonal to all the resonance vectors $D_k$. These integrals commute with all the integrals of the unperturbed system and, therefore with the normalised Hamiltonian $H$ (Gustavson 1966). In the operator notation, for any analytic function $\hat{F}(x)$:

$$\hat{I}_m = \hat{\beta}_m \hat{I}_m, \quad m = 1, \ldots, d - r,$$

$$[\hat{I}_m, \hat{\beta}_m \hat{F}] = 0,$$

$$[\hat{I}_m, \hat{H}] = 0.$$

After the transform back to the initial variables, the quantities

$$I_m = \hat{U}_w^{-1} \hat{I}_m, \quad m = 1, \ldots, d - r,$$

become formal integrals of the perturbed system. These Gustavson integrals belong to the image of $\hat{P}_H$ and commute with all the functions in this space:

$$I_m = \hat{U}_w^{-1} \hat{P}_H \hat{I}_m = \hat{P}_H \hat{U}_w^{-1} \hat{I}_m = \hat{P}_H I_m, \quad m = 1, \ldots, d - r,$$

$$[I_m, \hat{P}_H F] = \overline{\hat{U}}_w^{-1} [I_m, \hat{P}_H \hat{U}_w F] = 0,$$

$$[I_m, \hat{H}] = \overline{\hat{U}}_w^{-1} [\hat{I}_m, \hat{H}] = 0.$$

Here, we have again used the intertwining of the projectors (10). Due to the above properties, the derivative of $I_m(x, \epsilon)$ does not depend on the $\hat{P}_H F$ part of $W$:

$$\frac{d}{d \epsilon} I_m(\epsilon) = \left( \frac{\partial}{\partial \epsilon} \overline{\hat{U}}_w^{-1} \right) I_m = -\hat{L}_W \overline{\hat{U}}_w^{-1} I_m = -\hat{L}_W I_m = -\hat{L}_W \delta_{ij} \delta_{ij} \epsilon I_m.$$

Therefore, the Gustavson formal integrals $I_m(\epsilon)$ are insensitive to the uniqueness condition. The corresponding series diverge (Contopoulos et al 2003), but are useful for exploring the regularity of dynamics.

The unperturbed Hamiltonian $H_0$ can be chosen as the initial function for the Gustavson integral. The resulting series is known as the Hori formal first integral (Hori 1966):

$$I_H = -\epsilon^3 \left( H - \overline{\hat{U}}_w^{-1} \delta_{ij} \partial_{ij} \epsilon H_0 \right) = \hat{P} H_1 + \epsilon \left( \hat{P} H_2 - \hat{S} L_{H_1} \hat{P} H_1 - \frac{1}{2} \hat{P} L_{H_1} \hat{S} H_1 \right)$$

$$+ \epsilon^2 \left( \hat{S} L_{H_1} \hat{P} H_1 + \frac{1}{2} \hat{S} \hat{L}_{H_1} \hat{P} \hat{H}_1 + \frac{1}{3} \hat{P} L_{H_1} \hat{S} L_{H_1} \hat{S} H_1 - \frac{2}{3} \hat{P} L_{H_1} \hat{S}^2 L_{H_1} \hat{P} H_1 \right.$$  

$$- \frac{1}{2} \hat{P} L_{H_1} \hat{P} L_{H_1} \hat{S}^3 H_1 - \hat{S} L_{H_1} \hat{P} H_2 - \hat{S} L_{H_1} \hat{P} H_2 + \hat{P} H_3 \right) + O(\epsilon^3).$$

It is also applicable to systems with non-constant unperturbed frequencies.
6 Computational aspects

A major difference between this and the classical canonical perturbation algorithms is the explicit non-recursive formulae. Usually, perturbation computations normalise the Hamiltonian order by order. In contrast, we compute the generator up to the desired order directly. Next, the direct Lie-Deprit transform normalises the perturbed Hamiltonian, and the inverse transform computes its integrals.

6.1 An explicit algorithm for the generator

To normalise the Hamiltonian \( H \) up to the order \( O(\varepsilon^{N+1}) \), we must compute the generator \( W \) up to \( O(\varepsilon^N) \). It is possible, but not efficient, to use the combinatorial sum \( (22) \). A more elegant algorithm follows from the Neumann series \((14)\). Consider the following expression:

\[
\hat{R}_H(z) \frac{\partial H}{\partial \varepsilon} = \hat{R}_H(z) \sum_{n=0}^{N-1} (-L^\varepsilon \hat{R}_H(z)) \frac{\partial H}{\partial \varepsilon} + O(\varepsilon^N),
\]

where \( V = \sum_{k=1}^{N-1} \varepsilon^k H_k \).

Its coefficient of \( z^0 \) gives the generator \( W = \hat{S}_H \frac{\partial H}{\partial \varepsilon} \) up to the desired accuracy.

In order to avoid the negative powers of the ancillary variable \( z \) during computation, we use the operator:

\[
\hat{Q}(z) = -\hat{P}_H + \sum_{n=1}^{N} \varepsilon^n \hat{S}_H^n \equiv z \hat{R}_H(z) + O(z^{N+1}).
\]

In the Birkhoff representation, the action of this linear operator on a monomial is computed as follows:

\[
\hat{Q} \varepsilon^k \eta^m = \begin{cases} 
- \varepsilon^k \eta^m, & \text{when } (\omega, k - m) = 0, \\
\sum_{n=1}^{N} \left( \frac{1}{1/2(k - m)} \right)^n \varepsilon^k \eta^m, & \text{when } (\omega, k - m) \neq 0.
\end{cases}
\]

The expression in the action-angle variables is similar.

Our algorithm sequentially constructs the \( N - 1 \) functions:

\[
F_1(x, \varepsilon, z) = \hat{Q} \frac{\partial H}{\partial \varepsilon}, \quad \ldots, \quad F_n(x, \varepsilon, z) = -\hat{Q} \hat{L}_V F_{n-1}, \quad n = 1, \ldots, N.
\]

At each step, a computer algebra system automatically discards all the terms containing \( \varepsilon^N \) and \( z^{N+1} \). The generator up to \( O(\varepsilon^N) \) is directly computed from these functions:

\[
W(\varepsilon) = \hat{S}_H \frac{\partial H}{\partial \varepsilon} = \sum_{n=1}^{N} F_n[\varepsilon^n],
\]

where \( F_n[\varepsilon^n] \) denotes the coefficient of \( \varepsilon^n \) in the function \( F_n(x, \varepsilon, z) \).

\footnote{The rational expression \( z/(\iota(\omega, k - m) - z) \varepsilon^k \eta^m \) is preferable for some computer algebra systems.}
6.2 Computation of the Lie-Deprit transforms

Traditionally, the Lie-Deprit transform $\hat{U}$ and the generator $W$ are simultaneously computed order by order using the triangular algorithm (Deprit 1969). In our approach, we compute the generator independently and can use faster algorithms.

The inverse transform: Let us first consider the Gustavson integrals $I_m(x,\varepsilon)$. These quantities are computed by the application of $\hat{U}_W^{-1}$ to the quantities $\tilde{I}_m(x)$ that do not depend on $\varepsilon$. An efficient computation should utilize this property (Henrard 1973).

The Henrard algorithm is based on the recursive relation \( (8) \). In our particular case, it iteratively constructs $N+1$ ancillary functions:

\[
\tilde{f}_0 = \tilde{I}_m(x), \quad \ldots, \quad \tilde{f}_n = -\frac{1}{n} \sum_{k=0}^{n-1} \hat{L}_{W_{n-k}} \tilde{f}_k, \quad n = 1, \ldots, N.
\]

These functions are the coefficients of the approximation for the Gustavson integral:

\[
I_m(x,\varepsilon) = \hat{U}_W^{-1} I_m = \sum_{n=0}^{N} \varepsilon^n \tilde{f}_n + O(\varepsilon^{N+1}).
\]

The direct transform: Inspired by the simplicity and the efficiency of the above computation, we propose a similar algorithm for the direct Lie-Deprit transform. The normalised Hamiltonian can be written as the following sum:

\[
\tilde{H} = \hat{U}_N H = \left( \sum_{n=0}^{N} \varepsilon^n \hat{U}_n \right) \left( \sum_{n=0}^{N} \varepsilon^n H_n \right) + O(\varepsilon^{N+1}) = \sum_{n=0}^{N} \hat{U}_n f^{(N)}_n + O(\varepsilon^{N+1}).
\]

Here, we introduce the ancillary double-indexed functions $f^{(N)}_n(x,\varepsilon) = \sum_{k=0}^{n} \varepsilon^k H_{k-n}$.

The relations \( (8) \) allows us repeatedly express the operators $\hat{U}_n$ by means of $\hat{U}_{\text{less than } n}$:

\[
\tilde{H} = \hat{U}_N f^{(N)}_N + \sum_{k=0}^{N-1} \hat{U}_k f^{(N)}_k = \sum_{k=0}^{N-1} \hat{U}_k f^{(N-1)}_k = \ldots = \sum_{k=0}^{n} \hat{U}_k f^{(n)}_k = \ldots,
\]

where the functions $f^{(n)}_k, n = N-1, \ldots, 0$ are computed using the relations:

\[
f^{(n)}_k = f^{(n+1)}_k + \frac{1}{n+1} \hat{L}_{W_{n-k}} f^{(n+1)}_{n+1}, \quad k = 0, \ldots, n.
\]

Finally, all the operators $\hat{U}$ disappear and we obtain the transformed Hamiltonian:

\[
\tilde{H} = \ldots = f^{(1)}_0 + \hat{U}_1 f^{(1)}_1 = f_0^{(0)}.
\]

The functions $f^{(n)}_k(x,\varepsilon)$ form a triangle similar to that of Deprit, but their computation does not include the summation.
7 Examples and comparison with other canonical algorithms

In the following examples, we compare the normalisation of the model Hamiltonians using our explicit algorithm with the results of the major canonical perturbation approaches, including Gustavson (1966), Hori-Mersman (1970), Henrard (1973) and Dragt and Finn (1976) algorithms.

7.1 Pendulum

The Hamiltonian of the standard one-dimensional pendulum is \( P^2/2 + (1 - \cos Q) \). The canonical non-univalent scale transform \( P = \sqrt{\epsilon} p, \ Q = \sqrt{\epsilon} q \) allows us to introduce the perturbation parameter:

\[
H = \frac{1}{2} (p^2 + q^2) + \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{(2(k + 1))!} q^{2(k+1)} \epsilon^k.
\]

The first orders of the normalising generator and the normalised Hamiltonian are:

\[
W = \frac{5}{192} p_1 q_1^3 + \frac{1}{64} p_1^3 q_1 + \epsilon \left( \frac{17}{7680} p_1^5 q_1^5 + \frac{1}{192} p_1^3 q_1^3 + \frac{1}{512} p_1^5 q_1 \right) + O(\epsilon^3),
\]

\[
\tilde{H} = \frac{1}{2} (p^2 + q^2) - \frac{1}{64} (p^2 + q^2)^2 \epsilon - \frac{1}{2048} (p^2 + q^2)^3 \epsilon^2 - \frac{5}{131072} (p^2 + q^2)^4 \epsilon^3
\]

\[
- \frac{33}{8388608} (p^2 + q^2)^5 \epsilon^4 - \frac{63}{134217728} (p^2 + q^2)^6 \epsilon^5 + O(\epsilon^6).
\]

This is the typical structure of the perturbation series for non-resonance systems. Although different canonical perturbation methods build different near-identity canonical normalising transforms, the normalised Hamiltonians of non-resonance systems are identical (Koseleff 1994).

7.2 Toda 2D system

The Toda two-dimensional system has the following Hamiltonian:

\[
H_T = \frac{1}{2} (p_1^2 + p_2^2) + \frac{1}{24} \left( e^{2Q_1} + e^{2Q_2} + e^{2Q_1} + e^{2Q_2} \right) + \frac{1}{8}.
\]

Its integrability was first stated by Ford et al (1973) using perturbative method.

The scale transform \( P_j = \epsilon p_j, \ Q_j = \epsilon q_j \) introduces the perturbation parameter. It is worth mentioning that the first two orders of an \( \epsilon \) expansion for the Toda 2D system coincide with the Henon-Heiles Hamiltonian:

\[
H = \frac{1}{2} (p_1^2 + q_1^2 + p_2^2 + q_2^2) + \epsilon \left( -\frac{3}{2} q_1^2 + q_1^2 q_2 + \frac{1}{2} q_1^2 \right) + \epsilon^2 \left( \frac{11}{45} q_1^2 + \frac{1}{3} q_1^4 - \frac{1}{5} q_1^6 \right) + O(\epsilon^3).
\]
Because this is a 1:1 resonance system, the corresponding normalised Hamiltonian contains mixed terms, such as $\xi_1\eta_2$:

$$
\hat{H} = i(\xi_2\eta_2 + \xi_1\eta_1) + \epsilon^2 \left( -\frac{1}{3} \xi_2^2 \eta_2^2 + \frac{1}{3} \eta_2^2 \xi_2^2 - \frac{4}{3} \xi_1 \eta_1 \xi_2 \eta_2 + \frac{4}{3} \xi_1^2 \eta_1^2 - \frac{1}{3} \xi_1^2 \eta_1^2 \right) + i\epsilon^4 \left( -\frac{5}{27} \xi_2^3 \eta_2^3 - \frac{7}{9} \eta_2^3 \xi_2^3 + \xi_1 \eta_1 \xi_2 \eta_2^3 - \frac{7}{9} \xi_1 \eta_1 \xi_2 \eta_2^3 - \frac{5}{9} \xi_2^3 \eta_2^3 \right) + \xi_2^3 \eta_2^2 - \frac{7}{9} \xi_1 \eta_1 \xi_2 \eta_2^3 - \frac{5}{27} \xi_1^3 \eta_1^3 + O(\alpha^6).
$$

The following shows the series for the Gustavson integral:

$$
I_H = \epsilon^2 (H - \hat{H}) = \frac{1}{12} q_1^4 + \frac{1}{6} p_1^2 q_2^2 + \frac{1}{12} p_1^4 + \frac{1}{6} q_1^2 \eta_2^2 + \frac{1}{6} q_1^2 \eta_2^2 + \frac{1}{12} q_1^4 - \frac{2}{3} p_1 q_1 p_2 q_2 + \frac{1}{2} p_1^2 p_2^2 + \frac{1}{6} p_1^2 q_1^2 + \frac{1}{12} p_1^4 + \epsilon \left( -\frac{1}{9} q_2^4 - \frac{1}{9} p_2^4 + \frac{5}{3} q_1^2 p_2^2 + \frac{1}{3} q_1^2 q_2^2 - \frac{2}{3} p_1 q_1 p_2 q_2 + \frac{4}{3} p_1^3 q_1 p_3^3 \right) - \frac{2}{3} p_1^3 q_1^3 + \frac{7}{3} q_1^3 q_2^3 + \frac{4}{3} q_1^3 q_2^3 + \frac{4}{3} p_1^3 q_1^3 + \frac{4}{3} q_1^3 q_2^3 + \frac{4}{3} q_1^3 q_2^3 + \frac{4}{3} q_1^3 q_2^3 + O(\alpha^2).
$$

Again, the canonical perturbation methods build different near-identity canonical $\epsilon$-parametrized normalising transforms. The Gustavson (1966) method uses the generating functions of mixed variables according to Poincaré-Birkhoff-Von Zeipel approach. For the same purpose, the Hori-Mersman (1970) algorithm uses the Lie series (Magnus expansion), while Dragt and Finn (1976) construct a product of operatorial exponents (Fer expansion). The Deprit (1969) method builds the direct Lie-Deprit transform for the Hamiltonian normalisation, but its uniqueness condition differs from our explicit formula (21). Finally, the Henrard (1973) algorithm is based on the inverse Lie-Deprit transform. Traditionally, all these methods construct a non-secular generator.

All these normalising transforms are equivalent to the Lie-Deprit transforms with different uniqueness conditions $\mathbf{P}_\mu \mathbf{F}$. Because of the non-commutativity of the unperturbed integrals, the Hamiltonians of a resonance system normalised by different methods differ from each other.

As can be seen from our supplemental demonstrations, the normalised Toda 2D Hamiltonians constructed by the Deprit, Hori, Gustavson, Dragt-Finn and Henrard methods using the non-secular uniqueness condition differ from each other starting from the 8th order. All of them are connected by secular canonical transforms.

Moreover, we can either normalise the Hamiltonian in the $(p, q)$ variables or transform it first to the $(\eta, \zeta)$ variables, normalise it there and transform back. The results of the Lie algebraic algorithms are equal. Since the generating functions are not invariant under canonical transforms, the results of the Gustavson normalisations in the $(p, q)$ and $(\eta, \zeta)$ variables differ starting from the 6th perturbation order.

As expected, the series for the Gustavson integrals for all the methods coincide up to the highest order that we computed.
Henrard method: It is interesting that the Hamiltonian normalised by our explicit method coincides with that constructed by the Henrard (1973) method. This is not occasional. The Henrard method uses the fact that any direct Deprit transform $\hat{U}_W$ may be written as an inverse Deprit transform $\hat{U}_W^{-1}$ with the generator $\hat{W} = -\hat{U}_W W$.

The Henrard method normalises the perturbed Hamiltonian using this inverse Deprit transform because it is easier to compute. It constructs the generator $\hat{W}(x, \varepsilon)$ order by order using the requirement that $\hat{H} = \hat{U}_W^{-1} \hat{H} \hat{U}_W$ is secular. At each order it chooses the non-secular solution of the homological equation, therefore $\hat{P}_H \hat{W} \equiv 0$. The details can be found in Koseleff (1994).

Due to the intertwining relations (10):

$$\hat{P}_H \hat{W} = -\hat{P}_H \hat{U}_W W = -\hat{U}_W \hat{P}_H W \equiv 0,$$

the corresponding Deprit generator obeys our natural uniqueness condition $\hat{P}_H W \equiv 0$. Thus, the Henrard transform actually coincides with the Deprit transform with the generator obtained by the explicit formula (21).

8 Computational efficiency

Traditionally, the efficiencies of the perturbation methods are compared by the number of Poisson brackets (Broer et al 2003). However, this formal comparison does not take into account the resource consumption for solutions of homological equations, series substitution and memory management. This is why we prefer a computer benchmarking of the particular realisations of algorithms.

Unfortunately, even the benchmarking efficiency is not unambiguous. High-order computations process large multi-gigabyte expressions containing millions of terms. The performance of operations with such expressions depends on the computer algebra system used, optimisations, the server CPU, RAM, OS, disks and filesystem type. Even the relative efficiencies of the methods may vary. Therefore, the following results are only illustratory.

![Fig. 1: Hénon-Heiles system](image-url)
Figure 1 compares the times to compute the normalised Hamiltonian and the Gustavson integral for the Henon-Heiles system

\[ H_{HH} = \frac{1}{2}(p_1^2 + q_1^2 + p_2^2 + q_2^2) + \alpha (q_1^3 q_2 - \frac{1}{3}q_1^3) \]

on an Oracle™ Exadata X2-2 server with Intel Xeon X5675 (3.06 GHz) processor using Form 4.1 computer algebra system (Kuipers et al 2013). The Gustavson, Dragt-Finn and Henrad algorithms were run in the \((p, q)\) variables. The other methods have the better performance in the \((\eta, \zeta)\) variables.

We see that for a simple Hamiltonian with a limited number of perturbation terms only the Dragt-Finn and Henrad methods are faster than the explicit algorithm.

However, this changes for large Hamiltonians. For example, the number of terms up to the 32nd order in the Toda 2D Hamiltonian exceeds 36000 in the \((\eta, \zeta)\) variables. Corresponding computational times are presented in Figure 2. We see that our non-recursive explicit method becomes slower than the recursive Lie algebraic algorithms for high-order normalisation of such Hamiltonians.

Fig. 2: Toda 2D system

In all the cases we observed that the Dragt-Finn method had the superior performance. The Gustavson algorithm was the slowest for high-orders computations. Its time is dominated by the consecutive series substitutions during the integral computation.

It is worth noting that the computations were single-threaded. However, the explicit algorithm can be readily parallelized and made scalable for contemporary multi-CPU and Cloud computing.

9 Summary

We have presented the application of the Kato perturbation expansion for the Laurent coefficients of the Liouvillian resolvent to classical Hamiltonians represented
by a power series in a perturbation parameter. This generalises our previous results
(Nikolaev 2015) concerning the canonical intertwining of perturbed and unperturbed
averaging operators and the explicit expression for the generator of the normalising
Lie-Deprit transform in any perturbation order.

The approach allows for the systematic description of non-uniqueness in the gen-
erator and normalised Hamiltonian. We have also discussed the uniqueness of the
Gustavson integrals and compared the computational efficiency of the explicit expres-
sion for the Hénon-Heiles and the Toda 2D systems with the efficiencies of classical
canonical perturbation methods up to the 32nd perturbation order.

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