Kato perturbation expansion in classical mechanics and an explicit expression for a Deprit generator.

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Abstract. This work explores the structure of Poincare-Lindstedt perturbation series in Deprit operator formalism and establishes its connection to Kato resolvent expansion. A discussion of invariant definitions for averaging and integrating perturbation operators and their canonical identities reveals a regular pattern in a Deprit generator. The pattern was explained using Kato series and the relation of perturbation operators to Laurent coefficients for the resolvent of Liouville operator.

This purely canonical approach systematizes the series and leads to the explicit expression for the Deprit generator in any perturbation order:

\[ G = -\hat{S}_H H_i. \]

Here, \( \hat{S}_H \) is the partial pseudo-inverse of the perturbed Liouville operator. Corresponding Kato series provides a reasonably effective computational algorithm.

The canonical connection of perturbed and unperturbed averaging operators allows for a description of ambiguities in the generator and transformed Hamiltonian, while Gustavson integrals turn out to be insensitive to normalization style. Non-perturbative examples are used for illustration.

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1. Introduction.

This work was inspired by remarkable analogies between mathematical formalisms of perturbation expansions in classical and quantum mechanics. For instance, classical secular perturbation theory \cite{1} corresponds to time-dependent quantum mechanical perturbation expansion \cite{2}. “Action-angle” variables correspond to energy representation in quantum mechanics. The classical Poincare-Lindstedt method \cite{3} in Lie algebraic formalism \cite{4,5} has a direct analogy in quantum Van Vleck perturbation expansion \cite{6,7,8}. Similarly, classical Birkhoff-Gustavson normal forms relate to quantum mechanical perturbation theory in Bargmann-Fock space \cite{9,10}.

However, quantum mechanics has a wider diversity of perturbation methods. Some of these methods may be of interest for classical perturbation theory. Here we will construct a classical analogue of Kato series \cite{11}.
Kato used the Laurent and Neumann expansions of a resolvent operator around the eigenvalues of the quantum mechanical Hamiltonian. In classical mechanics, our tools will be the Liouville operator and its resolvent. But the spectrum of classical Liouvillian is more complex than that of quantum Hamiltonian [12]. Also, the multidimensional classical perturbation series must diverge on everywhere dense set of resonances [13].

Despite this internal divergence, canonical perturbation expansion is an efficient tool in celestial mechanics [14], nonlinear physics and accelerator theory. This is why new perturbative algorithms are important. We focus here on formal constructions of canonical perturbation series and general formulae. Their convergence and nonresonance cancellations will be discussed in another article.

It is worth noting that noncanonical perturbation expansions of Liouvillian resolvents were used by the Brussels-Austin Group in nonequilibrium statistical mechanics [15]. However, we will construct purely canonical series.

This paper is organized as follows. First, we review the construction of Poincaré-Lindstedt-Deprit series using invariant operator formalism and introduce convenient notation borrowed from quantum mechanics. We then discuss algebraic properties of basic perturbation operators. A set of canonical identities uncovers regular pattern in Deprit generator.

To extend this pattern to all orders, we borrow Abel averaging from quantum mechanics and establish a connection to the resolvent of Liouville operator and Kato expansion. Canonical properties of Liouvillian resolvent allow us to write a simple explicit expression for Deprit generator:

\[ G = -\hat{S}_H H. \]

In this formula, the integrating operator \( \hat{S}_H \) is the partial pseudo-inverse of the perturbed Liouville operator.

After providing a description of the generator structure in any perturbation order and its ambiguity and difference in normalization style from the standard Deprit algorithm, we will extend the formulae to a multidimensional case and discuss Gustavson integrals and computational efficiency. Finally, we will illustrate the findings using non-perturbative examples.

Our method combines classical and quantum mechanical perturbation approaches. The novel results are the observation of a regular pattern in the perturbation series for the generator, its explanation using Kato series, the explicit expression for Deprit generator in all perturbation orders and the insensitivity of Gustavson integrals to normalization style.

The “Supplementary data files” contain demonstrations and large formulae, including the general normal form of Hamiltonian up to the seventh perturbation order. The demonstrations use the freeware computer algebra system FORM [16].
2. Classical perturbation expansion.

2.1. Liouville operator.

Equations of motion, for most dynamical systems, cannot be solved analytically. Therefore, we should be interested in approximations that preserve underlying physical structures. One such approximation is the classical perturbation theory \cite{13}. It explores the dynamical behaviour of \(d\)-dimensional mechanical system with Hamiltonian, which differs from the solvable (integrable) system by the small perturbation

\[
H = H_0 + \alpha H_i,
\]

where \(H_0\) and \(H_i\) are the functions of canonical variables \(\vec{p}, \vec{q}\) on \(\mathbb{R}^d \times \mathbb{R}^d\). We will consider only autonomous (time-independent) Hamiltonians having compact energy surfaces \(H(\vec{p}, \vec{q}) = E\). We also assume that all functions are analytic.

Perturbation theory approximates the time evolution of canonical variables and constructs integrals of motion for perturbed system. More generally, it approximates the time evolution of function \(F(\vec{p}, \vec{q})\), obeying Hamiltonian equations:

\[
\frac{dF}{dt} = [F, H], \quad [F, H] = \sum_{i=1}^{d} \frac{\partial F}{\partial q_i} \frac{\partial H}{\partial p_i} - \frac{\partial F}{\partial p_i} \frac{\partial H}{\partial q_i}.
\]

Such evolution defines the continuous one-parametric family of canonical transformations of the phase space named \textit{Hamiltonian flow}. Using Liouville operator

\[
\hat{L}_H = [\cdot, H], \quad \hat{L}_H F = [F, H],
\]

the formal solution of Hamiltonian equations for an autonomous Hamiltonian may be written as operator exponent

\[
\tilde{F}(p, q)\bigg|_t = e^{t\hat{L}_H} F(p, q)\bigg|_0, \quad \hat{L}_H e^{t\hat{L}_H} = e^{t\hat{L}_H} \hat{L}_H. \tag{1}
\]

This is a canonical transformation commutative with the autonomous \(\hat{L}_H\).

2.2. Near-identity canonical transformations.

Classical perturbation theory uses a more general construction of a family of near-identity \(\alpha\) dependent canonical transformations on \(\mathbb{R}^{2d}\) phase space

\[
\tilde{x} = \hat{U}(\alpha)x, \quad \begin{cases}
x_i &= q_i, \\
x_{i+d} &= p_i,
\end{cases} \quad i = 1, \ldots d,
\]

equipped with the canonical structure

\[
[F(x), G(x)] = \sum_{i,j}^{2d} \frac{\partial F}{\partial x_i} \omega_{ij} \frac{\partial G}{\partial x_j}.
\]
Here, $\omega_{ij} = -\omega_{ji}$ is the non-degenerate skew-symmetric Jacobi matrix. Such canonical transformations are always Hamiltonian flows \[1, 17\]

$$\frac{\partial \hat{U}}{\partial \alpha} = \hat{L}_G \hat{U}$$

in “time” $\alpha$ with some generator $G(x, \alpha)$. The perturbation theory constructs this generator as the power series $G(x, \alpha) = \sum_0^\infty \alpha^n G_n(x)$. It also computes the series for the transformation $\hat{U} = \sum_0^\infty \alpha^n \hat{U}_n$ and its inverse, $\hat{V} = \hat{U}^{-1}$, which satisfies the equation

$$\frac{\partial \hat{V}}{\partial \alpha} = -\hat{V} \hat{L}_G.$$  \hspace{1cm} (2)

In celestial mechanics these formulae are known as “Lie transforms” by Deprit \[4\]. Substituting series for $G$, $\hat{U}$ and $\hat{V}$ into the above equations, Deprit obtained the recursive relations for coefficients:

$$\hat{U}_n = \frac{1}{n} \sum_{k=0}^{n-1} \hat{L}_{G_{n-k-1}} \hat{U}_k, \quad \hat{V}_n = -\frac{1}{n} \sum_{k=0}^{n-1} \hat{V}_k \hat{L}_{G_{n-k-1}}.$$  \hspace{1cm} (3)

These expressions can be iterated to derive the non-recursive formulae \[1, 18\]

$$\hat{U}_n = \sum_{(m_1, \ldots, m_r)} \frac{\hat{L}_{G_{n-m_1}} \hat{L}_{G_{m_2-m_1}} \cdots \hat{L}_{G_{m_r-1}}}{m_1 \cdots m_r},$$

$$\hat{V}_n = \sum_{(m_1, \ldots, m_r)} (-1)^{r+1} \frac{\hat{L}_{G_{m_r-1}} \hat{L}_{G_{m_2-m_1-1}} \cdots \hat{L}_{G_{n-m_1-1}}}{m_1 \cdots m_r}.$$  \hspace{1cm} (4)

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

Hereafter, we will use the notation $\hat{U} = \exp_D(\alpha \hat{L}_G)$, $\hat{V} = \exp_D^{-1}(\alpha \hat{L}_G)$ and term “Deprit exponents” for these series to emphasize their exponential-like role. Look at the first few orders:

$$\exp_D(\alpha \hat{L}_G) = 1 + \alpha \hat{L}_G + \frac{\alpha^2}{2}(\hat{L}_G^2 + \hat{L}_G)$$

$$+ \frac{\alpha^3}{6}(\hat{L}_G^3 + \hat{L}_G \hat{L}_G + 2\hat{L}_G \hat{L}_G + 2\hat{L}_G) + O(\alpha^3)$$

$$\exp_D^{-1}(\alpha \hat{L}_G) = 1 - \alpha \hat{L}_G + \frac{\alpha^2}{2}(\hat{L}_G^2 - \hat{L}_G)$$

$$- \frac{\alpha^3}{6}(\hat{L}_G^3 - 2\hat{L}_G \hat{L}_G - \hat{L}_G \hat{L}_G + 2\hat{L}_G) + O(\alpha^3)$$  \hspace{1cm} (5)

See also “deprit_exponents” demo in the supplementary data files.

We will outline here the key properties of canonical transformation $\hat{U}$. This is the point transformation of phase space $\hat{U} F(x) = F(\hat{U} x)$, which also preserves Poisson brackets. It make sense to consider the Poisson bracket as an additional antisymmetric
Kato perturbation expansion in classical mechanics

product (Poisson algebra). Canonical transformations preserve both the algebraic and canonical structures of function space

\[
\hat{U}(FH) = (\hat{U}F)(\hat{U}H),
\]

\[
\hat{U}([F, H]) = [\hat{U}F, \hat{U}H],
\]

for any functions \(F(x)\) and \(H(x)\).

Due to the Leibniz rule and Jacobi identity, the Liouville operator is the “derivation” of both products

\[
\hat{L}_G(FH) = (\hat{L}_G F)H + F(\hat{L}_G H),
\]

\[
\hat{L}_G[F, H] = [\hat{L}_G F, H] + [F, \hat{L}_G H].
\]

This dialgebraic property will be used to establish identities for perturbation operators.

The operator formalism of generators, or Lie-algebraic approach, was introduced in the perturbation theory of classical mechanics in 1966 [19]. This formalism is much simpler for computer algebra calculations than the previous ones that use generating functions. It is interesting that corresponding quantum mechanical formalism [6] appeared more than 40 years before its classical analogue.

Our goal is to transform canonically the perturbed Hamiltonian into a simpler, preferably integrable form. The transformed Hamiltonian will become an integral of motion of the unperturbed system. Here we briefly review this standard construction.

The canonical map \(\tilde{x} = \exp_D(\alpha \hat{L}_G) x\) transforms the perturbed Hamiltonian into

\[
\tilde{H} = \exp_D^{-1}(\alpha \hat{L}_G)(H_0 + \alpha H_i) = H_0 + \alpha(H_i - \hat{L}_{G_0} H_0) + O(\alpha^2)
\]

\[
= H_0 + \alpha(\hat{L}_{H_0} G_0 + H_i) + \frac{\alpha^2}{2}(\hat{L}_{H_0} G_1 + \hat{L}^2_{G_0} H_0 - 2\hat{L}_{G_0} H_i) + O(\alpha^3). \tag{4}
\]

To simplify coefficients, one needs to invert the Liouville operator \(\hat{L}_{H_0}\). Since this operator has a non-empty kernel, only its pseudo-inverse can be constructed.

2.3. Basic perturbation operators.

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 [13]. The time average

\[
\langle F \rangle = \lim_{T \to \infty} \frac{1}{T} \int_0^T F(\vec{p}(t), \vec{q}(t))|_{p(0)=p, q(0)=q} \, dt = \lim_{T \to \infty} \frac{1}{T} \int_0^T e^{i\hat{H}_0 t} F(x) \, dt \tag{5}
\]

exists in an “Action–Angle” representation for any analytic function \(F(x)\). This average is a function of the initial point \(x\). Being written in an invariant form, it also exists in other canonical variables.
The 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 ($C,1$) averaging [20]. Corresponding operator

$$\hat{P}_{H_0} = \lim_{T \to \infty} \frac{1}{T} \int_0^T dt \ e^{iH_0 t}$$

(6)

is projector $\hat{P}_{H_0}^2 = \hat{P}_{H_0}$. It projects $F(x)$ onto the secular space of functions commutative with $H_0$. This is the kernel of $\hat{L}_{H_0}$ and the algebra of its integrals of motion.

The notation $\hat{P}_{H_0}$ was borrowed from quantum mechanics. Standard notations like $\langle \rangle$, $F$ and $M_t$ [21, 22] do not emphasize the pattern in perturbation expansion that we seek.

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 here only semi-simple $\hat{L}_{H_0}$).

This inverse is the integrating operator $\hat{S}_{H_0}$, which is also known as the “solution of homological equation”, “tilde operation”, “zero-mean antiderivative” [23], “Friedrichs $\hat{G}$ operation” [24], “$1/k$ operator”, etc. Its invariant definition is [21]

$$\hat{S}_{H_0} = - \lim_{T \to \infty} \frac{1}{T} \int_0^T dt \int_0^t \ d\tau \ e^{i\tau H_0} \left(1 - \hat{P}_{H_0}\right).$$

(7)

See also [25, 26] for periodic extensions. The formal calculation

$$\hat{L}_{H_0} \hat{S}_{H_0} = - \lim_{T \to \infty} \frac{1}{T} \int_0^T dt \int_0^t \ d\tau \ \frac{\partial}{\partial \tau} e^{i\tau H_0} \left(1 - \hat{P}_{H_0}\right)$$

$$\quad = - \lim_{T \to \infty} \frac{1}{T} \int_0^T dt \left(e^{iH_0 t} - 1\right)\left(1 - \hat{P}_{H_0}\right) = 1 - \hat{P}_{H_0},$$

confirms that $\hat{S}_{H_0}$ is the partial pseudo-inverse of the unperturbed Liouville operator:

$$\hat{L}_{H_0} \hat{S}_{H_0} = \hat{S}_{H_0} \hat{L}_{H_0} = 1 - \hat{P}_{H_0},$$

$$\hat{S}_{H_0} \hat{P}_{H_0} = \hat{P}_{H_0} \hat{S}_{H_0} \equiv 0.$$

These three basic operators ($\hat{L}_{H_0}$, $\hat{P}_{H_0}$, $\hat{S}_{H_0}$) are the building blocks of perturbation expansion. Classical perturbation theory provides several algorithms to compute them:

- “Action-Angle” representation [13]. With its roots deep in the 19th century, it can be traced to Le Verrier and Delaunay. In “Action-Angle” canonical coordinates, the unperturbed Hamiltonian is the function of $d$ “action” variables $\vec{J}$ only, and the perturbation is $2\pi$ periodic in the phases $\vec{\phi}$

$$H = H_0(\vec{J}) + \alpha H_i(\vec{J}, \vec{\phi}) = H_0(\vec{J}) + \alpha \sum_{\vec{k}} \hat{H}_i(\vec{J}, \vec{k}) e^{i(\vec{k}, \vec{\phi})}.$$
The motion of an unperturbed system is quasi-periodic:
\[ \vec{J} = \text{const}, \quad \vec{\phi}(t) = \vec{\omega} t + \vec{\phi}_0, \quad \vec{\omega} = \frac{\partial H_0}{\partial \vec{J}}. \]

Because the Fourier components in the "Action-Angle" representation are eigenfunctions of \( \hat{L}_{H_0} \), the perturbation operators can be written as
\[
\hat{P}_{H_0} F = \lim_{T \to \infty} \frac{1}{T} \int_0^T dt \sum_k \tilde{F}(\vec{J}, \vec{k}) e^{i(\vec{k}, \vec{\phi}_0) + i(\vec{\omega}, \vec{k})t},
\]
\[
\hat{S}_{H_0} F = \sum_{(\vec{\omega}, \vec{k}) \neq 0} \frac{1}{i(\vec{\omega}, \vec{k})} \tilde{F}(\vec{J}, \vec{k}) e^{i(\vec{k}, \vec{\phi}_0)}.
\]

These well-known expressions are frequently used as the definitions of \( \hat{P}_{H_0} \) and \( \hat{S}_{H_0} \).

- **"Birkhoff-Gustavson-Bruno" normalization** \([27, 28, 29]\) for power series. In its simplest case, a quadratic unperturbed Hamiltonian is diagonalizable into
\[
H_0 = \sum \frac{\omega_k}{2} (p_k^2 + q_k^2).
\]

After the following canonical transformation to complex variables (analogs of \( \hat{a}, \hat{a}^\dagger \) in quantum mechanics),
\[
\begin{align*}
q_k &= \frac{1}{\sqrt{2}} (\xi_k + i \eta_k), \\
p_k &= \frac{i}{\sqrt{2}} (\xi_k - i \eta_k),
\end{align*}
\]
the Hamiltonian becomes
\[
H = \sum_{k=1}^d i \omega_k \xi_k \eta_k + \alpha \sum_{|\vec{m}|+|\vec{n}| \geq 3} \tilde{H}_i(\vec{m}, \vec{n}) \prod_{k=1}^d \xi_k^{m_k} \eta_k^{n_k}.
\]

The monomials \( \xi^{\vec{m}} \eta^{\vec{n}} = \prod \xi_k^{m_k} \eta_k^{n_k} \) are eigenvectors of the unperturbed Liouvillian
\[
\hat{L}_{H_0} \xi^{\vec{m}} \eta^{\vec{n}} = i(\vec{\omega}, \vec{m} - \vec{n}) \xi^{\vec{m}} \eta^{\vec{n}}.
\]

Therefore, for any series \( F(\vec{p}, \vec{q}) = \sum \tilde{F}(\vec{m}, \vec{n}) \xi^{\vec{m}} \eta^{\vec{n}} \):
\[
\hat{P}_{H_0} F = \sum_{(\vec{\omega}, \vec{m} - \vec{n}) = 0} F(\vec{m}, \vec{n}) \xi^{\vec{m}} \eta^{\vec{n}},
\]
\[
\hat{S}_{H_0} F = \sum_{(\vec{\omega}, \vec{m} - \vec{n}) \neq 0} \frac{1}{i(\vec{\omega}, \vec{m} - \vec{n})} F(\vec{m}, \vec{n}) \xi^{\vec{m}} \eta^{\vec{n}}.
\]

This is only a small excerpt from the greater area of normal form theory \([29, 23]\).

- **"Algebraic approaches."** \([30, 31]\) These solve the homological equation using matrix methods in the enveloping algebra.
• “Zhuravlev quadrature.” This directly integrates $F(x)$ along the unperturbed solution $x(t, x_0)$. The asymptotic of the single quadrature
\[
\int_0^T F(\vec{p}(t, \vec{q}_0, \vec{p}_0)), \vec{q}(t, \vec{q}_0, \vec{p}_0))dt, \quad T \to \infty
\]
contains both $\hat{P}_{H_0}F$ and $\hat{S}_{H_0}F$ inside its $O(T)$ and $O(1)$ parts, respectively. This quadrature is very efficient in normal form theory.

2.4. Deprit perturbation series.

If one chose $G_0 = -\hat{S}_{H_0}H_i$ in (4), then all terms of order $\alpha$ in the transformed Hamiltonian will become secular (begin with $\hat{P}_{H_0}$), as follows:
\[
\tilde{H} = \exp_D^{-1}(\alpha \hat{L}_G)(H_0 + \alpha H_i) = H_0 + \alpha \hat{P}H_i + \frac{\alpha^2}{2} \left( \hat{L}_{H_0}G_1 + \hat{L}_{S_{H_i}}(1 + \hat{P})H_i \right) + O(\alpha^3).
\]

Hereafter, we will omit the subscript $H_0$ for unperturbed $\hat{P}_{H_0}$ and $\hat{S}_{H_0}$ operators.

In the next orders, one can consequentially choose $G_1 = -\hat{S}_{\hat{L}_{S_{H_i}}}(1 + \hat{P})H_i$ to eliminate nonsecular terms up to $\alpha^2$, then $G_2$ to eliminate nonsecular terms up to $\alpha^3$ and so on. We will refer to this process as to the programme of classical Poincaré-Lindstedt perturbation theory: using near-identity canonical transformation, turn the Hamiltonian into an integral of the unperturbed system.

Compare this to quantum mechanical perturbation theory: using near-identity unitary transformation, turn the Hamiltonian operator into a block-diagonal form (commutative with the unperturbed Hamiltonian).

The described procedure recursively constructs a generator of normalizing transformation up to any order in $\alpha$. One may find details of “Deprit’s triangular algorithm” in classical books on perturbation theory. Here we will search for regularities in perturbation series. Look at the first few orders:
\[
G = -\hat{S}H_i - \alpha \hat{S}\hat{L}_{\hat{S}H_i}(1 + \hat{P})H_i - \alpha^2 \hat{S} \left( \frac{1}{2} \hat{L}_{\hat{S}H_i} \hat{L}_{\hat{P}H_i} \right) - \left( \hat{L}_{H_i} \hat{S} - \hat{L}_{\hat{S}H_i} \hat{P} + \frac{1}{2} \hat{L}_{\hat{P}H_i} \hat{S} \right) \hat{L}_{(1 + \hat{P})H_i} \right) \hat{S}H_i + O(\alpha^3)
\]
\[
\tilde{H} = H_0 + \alpha \hat{P}H_i + \frac{\alpha^2}{2} \hat{P} \hat{L}_{\hat{S}H_i}(1 + \hat{P})H_i + \frac{\alpha^3}{3} \hat{P} \left( \frac{1}{2} \hat{L}_{\hat{S}H_i} \hat{L}_{\hat{P}H_i} \right) \hat{L}_{(1 + \hat{P})H_i} \right) \hat{S}H_i + O(\alpha^3)
\]

At first glance, there is no notable pattern in the above expressions. However, in the subsequent sections of this work, they will be transformed into a more systematic form using canonical identities.

Obviously, the generator $G$ is not unique. An arbitrary secular function may be added to any order. Further orders will depend on this term. The rule for choosing the secular part of $G$ is called (hyper-)normalization style. Usually, one constructs
a completely nonsecular generator of Poincaré-Lindstedt transformation $\hat{P}_{H_0}G = 0$. However, we will see that other conditions may be useful.

It is now necessary to say a few words about the integrability of normalized system. In the non-resonant case, the unperturbed $d$-dimensional system has only $d$ integrals of motion. The normalized non-resonant Hamiltonian will be a function of these “actions” only, and are formally integrable (up to $O(\alpha^n)$).

However, if the unperturbed system has $r$ independent resonance relations $(\vec{\omega}, \vec{D}_k) = 0$, $k = 1, \ldots, r$, then it has $r$ additional non-commutative integrals. There still exists $d$ involutive actions, but normalized Hamiltonian will also depend on phases. Even in this resonant case, one can decrease the order of perturbed system by at least the dimension of center of the algebra of unperturbed integrals. This center consists of $d - r$ commutative with all other integrals [28]. Reduction by these variables [13, 36] results in an effective $r$ dimensional system. Therefore, in case that two or more resonances relations exist, the normalized system will be generally non-integrable.

Here is the difference between classical and quantum-mechanical perturbation theories. In quantum mechanics, one can always completely diagonalize a Hamiltonian with any number of resonant relations. Additional quantum integrals and the connection of diagonalizing transformation to nonlinear finite-dimensional Bogolyubov transformations were discussed in [10, 37].

3. Canonical identities.

In order to simplify expressions, we must list the algebraic properties of basic perturbation operators $\hat{L}$, $\hat{P}_{H_0}$ and $\hat{S}_{H_0}$:

- Invariant definitions of $\hat{P}$ and $\hat{S}$ operators (6, 7) immediately lead to identities

$$
\hat{P}_{H_0} = H_0, \quad \hat{S}_{H_0} = 0,
$$

$$
\hat{P}_{L_{H_0}} = L_{H_0} \hat{P} = 0,
$$

$$
\hat{S}_{L_{H_0}} = L_{H_0} \hat{S} = 1 - \hat{P}.
$$

- Because canonical transformation preserves algebraic and Poisson products (brackets), then for any functions $F(x)$, $G(x)$ and $H_i(x)$ the following hold:

$$
\hat{P}(F \cdot \hat{P}G) = (\hat{P}F) \cdot (\hat{P}G),
$$

$$
\hat{P}L_{\hat{P}_{H_i}} = L_{\hat{P}_{H_i}} \hat{P},
$$

$$
\hat{S}(F \cdot \hat{P}G) = (\hat{S}F) \cdot (\hat{P}G),
$$

$$
\hat{S}L_{\hat{P}_{H_i}} = L_{\hat{P}_{H_i}} \hat{S}.
$$

The first two identities demonstrate that the projector $\hat{P}$ preserves the products if one operand already belongs to the algebra of integrals of motion. This is the canonical analogue of orthogonal projection.
• Since $\hat{L}$ is the derivation for both algebraic and Poisson products of functions, there exists the integration by parts formulae known as Friedrichs identity \[24]\:

\[
\hat{S}L_{H_i}\hat{F} = \hat{F}P - \hat{F}P, \quad \hat{S}(F \cdot \hat{S}G) = \hat{P}F \cdot \hat{S}^2G + \hat{S}F \cdot \hat{S}G - \hat{P}F \cdot \hat{S}G - \hat{P}(\hat{S}F \cdot \hat{S}G) + \hat{S}(\hat{F}F \cdot \hat{P}G)
\]

The proof follows from an application of both sides of $\hat{S}L_{H_0} = 1 - \hat{P}$ to the product $\hat{L}_{H_i}\hat{S}F = [\hat{S}F, \hat{S}H_i]$ (or $\hat{S}F \cdot \hat{S}G$), and an expansion of the Jacobi identity. We may achieve complete symmetry denoting the algebraic product as an operator. Hereafter, we will even omit the identities for algebraic product, automatically assuming the existence of complementary identities.

• Further identities exist for products of three basic operators. For any function $H_i$:

\[
\hat{P}L_{H_i} \hat{P} = \hat{L}_{p_{H_i}} \hat{P}, \quad \hat{S}L_{H_i} \hat{P} = \hat{L}_{S_{H_i}} \hat{P}.
\]

These are the consequences of Poisson bracket invariance under canonical transformations

\[
\hat{P}L_{H_i} \hat{P}F = \lim_{T \to \infty} \frac{1}{T} \int_0^T dt e^{tH_0} [\hat{P}F, H_i] = \lim_{T \to \infty} \frac{1}{T} \int_0^T dt [e^{tH_0} \hat{P}F, e^{tH_0} H_i].
\]

Since $\hat{P}F$ is the integral of motion for $H_0$,

\[
\hat{P}L_{H_i} \hat{P}F = [\hat{P}F, \lim_{T \to \infty} \frac{1}{T} \int_0^T dt e^{tH_0} H_i] = \hat{L}_{p_{H_i}} \hat{P}F.
\]

The proof of the second identity is similar.

• The Burshtein-Soloviev identity \[38]\:

\[
\hat{P}L_{H_i} \hat{S} = \hat{S}L_{H_i} \hat{P},
\]

follows from identically zero expression $\hat{P}L_{H_0} \hat{S}H_i \hat{S} = 0$. Using the Jacobi identity $\hat{L}_F \hat{L}_G - \hat{L}_G \hat{L}_F = \hat{L}_{F \cdot G}$, we can write

\[
0 = \hat{P}L_{H_0} \hat{S}_{H_i} \hat{S} = \hat{P}L_{H_i} \hat{S}_{H_i} \hat{S} + \hat{P}L_{H_0} \hat{S}_{H_i} \hat{S} = \hat{P}L_{H_i} \hat{S}_{H_i} + \hat{P}L_{H_i} \hat{S} - \hat{P}L_{H_i} \hat{P} - \hat{P}L_{p_{H_i}} \hat{S}.
\]

Here the last two terms vanish, due to (14) and (12). Therefore, $\hat{P}L_{H_i} + \hat{P}L_{H_i} \hat{S} = 0$. The identities (11) – (15) is all that we need to simplify the Depriet series. They could be directly verified in an “Action-Angle” representation. Later we will find their generalization.

We have used the computer algebra system FORM \[16]\ to implement the above formulae. Due to canonical identities, the first orders of the Depriet series (10) have been
Kato perturbation expansion in classical mechanics

reduced to very inspiring form (see also the “deprit_series” demo):

\[ G = -\hat{S}H_i + \alpha \left( \hat{S}\hat{L}\hat{S}H_i - \hat{S}^2\hat{P}H_i \right) + \alpha^2 \left( -\hat{S}\hat{L}\hat{S}\hat{L}H_i \right. \\
\left. + \hat{S}\hat{L}\hat{S}\hat{P}H_i + \hat{S}^2\hat{L}\hat{L}\hat{P}H_i \right) + O(\alpha^3) \]

\[ \tilde{H} = H_0 + \alpha \hat{P}H_i - \frac{\alpha^2}{2} \hat{P}\hat{L}\hat{S}H_i + \alpha^3 \left( \frac{1}{3} \hat{P}\hat{L}\hat{S}\hat{L}H_i - \frac{1}{6} \hat{P}\hat{L}\hat{S}^2\hat{L}H_i \right) + O(\alpha^4) \]  

(16)

The expression for the transformed Hamiltonian corresponds to the classic result of Burshtein and Soloviev [38, 21]. In standard notation, this is

\[ \tilde{H} = H_0 + \alpha \hat{P}H_i + \frac{\alpha^2}{2} \left[ \hat{H}_i, \hat{H}_i \right] + \frac{\alpha^3}{3} \left[ \hat{H}_i, \left[ \hat{H}_i, \frac{\hat{H}_i + H_i}{2} \right] \right] + O(\alpha^4). \]

It is intriguing that the expression for \( G \) looks like a simple sum of all compositions of the \( -\hat{S} \) and \( \hat{P} \) operators. In the third order, the expression for the non-secular style Deprit generator loses this structure. Nevertheless, we observed that such sums actually normalize the Hamiltonian in the next orders. This should be explored further.

4. Kato expansion.

4.1. Resolvent of Liouville operator

Quantum mechanics commonly uses the stronger Abel averaging [20] procedure

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

This can also be applied to the classical case. Corresponding averaging and integrating operators are known from quantum mechanics [39, 40, 41]:

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

\[ \hat{S}_{H_0} = -\lim_{\lambda \to +0} \int_0^{\infty} dt \, e^{-\lambda t} e^{\lambda H_0} \left( 1 - \hat{P}_{H_0} \right). \]  

Whenever the Cesàro average [5] exists, Abel averaging gives the same results [20]. This is why we use the same notation. From this point, we will always assume Abel averaging, if not otherwise specified, as this greatly simplifies formulae and forms a natural connection to resolvent formalism. Strictly speaking, we should discuss corresponding Tauberian theorems, but we have limited our goal to formal expressions only.

The Abel averaging definitions for \( \hat{S}_{H_0} \) and \( \hat{P}_{H_0} \), as well as quantum mechanical analogies, suggest exploring the resolvent of Liouville operator

\[ \mathcal{R}_H(z) = \frac{1}{\lambda H - z}, \]  

(18)
This operator-valued function of the complex variable $z$ is the Laplace transform of the evolution operator of Hamiltonian system

$$\hat{\mathcal{R}}_H(z) = -\int_0^{+\infty} dt e^{-zt} e^{\hat{L}_H}.$$  

Resolvent singularities are the eigenvalues of $\hat{L}_H$. For integrable Hamiltonian system with compact energy surfaces, these eigenvalues belong to an imaginary axis. Typically, the spectrum of a Liouville operator is anywhere dense $[12]$. But let us begin with the simpler case of an isolated point spectrum. We will consider one-dimensional system and restrict the domain of resolvent operator to analytic functions with 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 points $0, \pm i \omega(E), \pm 2i \omega(E), \ldots$

We are interested in the analytical structure of the resolvent around zero. The existence of $\hat{P}_{H_0}$ and $\hat{S}_{H_0}$ means that the unperturbed resolvent has a simple pole in $0$. The averaging operator is the residue of the resolvent in this pole

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

while the integrating operator $\hat{S}_{H_0}$ is its holomorphic part

$$\hat{S}_{H_0} = \lim_{z \to 0} \hat{\mathcal{R}}_{H_0}(z)(1 - \hat{P}_{H_0}).$$

Therefore, the Liouvillian resolvent combines both basic perturbation operators $[12]$. We will also need the Hilbert identity,

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

which holds for any complex $z_1$ and $z_2$ outside of the spectrum (resolvent set) of $\hat{L}_H$.

The Laurent series. Despite the fact that the unperturbed resolvent has the simple pole in the origin, the perturbed resolvent may be more singular. The Laurent series of the resolvent with an isolated singularity in origin is

$$\hat{\mathcal{R}}_H(z) = \sum_{n=-\infty}^{+\infty} \hat{\mathcal{R}}^{(n)}_H z^{n-1}, \quad \hat{\mathcal{R}}^{(n)}_H = \frac{1}{2\pi i} \oint_{|z|=\epsilon} \hat{\mathcal{R}}_H(z) z^{-n} dz$$

(here $(n)$ is index).

It is well known that the Hilbert resolvent identity $[19]$ defines the structure of this series $[11]$. For further usage, it makes sense to repeat here this derivation. Consider the product of the two coefficients

$$\hat{\mathcal{R}}^{(m)}_H \hat{\mathcal{R}}^{(n)}_H = \left(\frac{1}{2\pi i}\right)^2 \oint_{|z_1|=\epsilon_1} \oint_{|z_2|=\epsilon_2} \hat{\mathcal{R}}_H(z_1)\hat{\mathcal{R}}_H(z_2) \frac{z_1^{-m} z_2^{-n}}{z_2 - z_1} dz_1 dz_2$$

$$= \left(\frac{1}{2\pi i}\right)^2 \oint_{|z_1|=\epsilon_1} \oint_{|z_2|=\epsilon_2} \frac{z_1^{-m} z_2^{-n}}{z_2 - z_1} \left(\hat{\mathcal{R}}_H(z_2) - \hat{\mathcal{R}}_H(z_1)\right) dz_1 dz_2.$$
Integration around the two circles $\epsilon_1 < \epsilon_2 < \omega$ gives
\[
\frac{1}{2\pi i} \oint_{|z_1| = \epsilon_1} \frac{z_1^{-m}}{z_2 - z_1} \, dz_1 = \eta_m z_2^{-m}, \quad \text{where } \eta_n = \begin{cases} 
1 & \text{when } n \geq 1, \\
0 & \text{when } n < 1,
\end{cases}
\]
\[
\frac{1}{2\pi i} \oint_{|z_2| = \epsilon_2} \frac{z_2^{-n}}{z_2 - z_1} \, dz_2 = (1 - \eta_n) z_1^{-n}.
\]

As a result, the resolvent operator coefficients obey
\[
\hat{R}_H^{(m)} \hat{R}_H^{(n)} = (\eta_m + \eta_n - 1) \hat{R}_H^{(m+n)}.
\]

For $n = m = 0$, this states that resolvent residue (with a minus sign) is the projector
\[
\hat{R}_H^{(0)} = -\hat{R}_H^{(0)} \hat{R}_H^{(0)} = -\hat{P}_H,
\]
and
\[
\hat{R}_H^{(n)} = \hat{S}_H^n, \quad n \geq 1,
\]
\[
\hat{R}_H^{(-n)} = -\hat{D}_H^n.
\]
\[
\hat{S}_H \hat{P}_H = \hat{P}_H \hat{S}_H \equiv 0, \quad \hat{S}_H \hat{D}_H = \hat{D}_H \hat{S}_H \equiv 0,
\]
\[
\hat{P}_H \hat{D}_H = \hat{D}_H \hat{P}_H = \hat{D}_H.
\]

Here, $\hat{D}_H$ is the eigennilpotent operator, which does not have an unperturbed analogue ($\hat{D}_{H0} \equiv 0$). Therefore, the Laurent series of the general Liouvillian resolvent around $z = 0$ has the form \([11]\)
\[
\hat{R}_H(z) = -\frac{1}{z} \hat{P}_H + \sum_{n=0}^{\infty} z^n \hat{S}_H^{n+1} - \sum_{n=2}^{\infty} z^{-n} \hat{D}_H^{n-1}, \quad (22)
\]
while the unperturbed resolvent consists only of
\[
\hat{R}_{H0}(z) = \sum_{n=0}^{\infty} \hat{R}_{H0}^{(n)} z^{n-1} = -\frac{1}{z} \hat{P} + \sum_{n=0}^{\infty} z^n \hat{S}_H^{n+1}
\]
(remember that we omit the subscript $H_0$).

Canonical structure of resolvent. Yet another identity of the Hilbert type relates the resolvent of the Liouville operator to the Poisson brackets. For any $z_1, z_2, z_3$ outside of the spectrum of $\hat{L}_H$ and functions $F$ and $G$ the following hold true:
\[
\hat{R}_H(z_1)[\hat{R}_H(z_2)F, G] + \hat{R}_H(z_1)[F, \hat{R}_H(z_3)G] - [\hat{R}_H(z_2)F, \hat{R}_H(z_3)G] = (z_1 - z_2 - z_3) \hat{R}_H(z_1)[\hat{R}_H(z_2)F, \hat{R}_H(z_3)G]. \quad (23)
\]
This is another integration by parts formula. It follows from the application of identical operator $\hat{R}_H(z_1)(\hat{L}_H - z_1) \equiv 1$ to Poisson bracket $[\hat{R}_H(z_2)F, \hat{R}_H(z_3)G]$ and the
expansion of the Jacobi identity. A complementary identity exists for the algebraic product.

We will use this canonical identity in the operator form

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

(24)

Its Laurent coefficients for the unperturbed resolvent contain all previous canonical identities \([11] - [15]\). For example, the coefficient of \(z_1^2\) is the Friedrichs identity \([13]\), and so on. Integrating \((24)\) like Hilbert identity before, we can obtain advanced identities. We will do this for a perturbed resolvent in the next chapter.

### 4.2. Kato series

The perturbed resolvent can be expanded into the Neumann series as follows:

\[ \mathcal{R}_{H_0 + \alpha H_1}(z) = \mathcal{R}_{H_0} - \alpha \mathcal{R}_{H_0} \hat{\mathcal{L}}_{\mathcal{R}_{H_0}} \mathcal{R}_{H_0} + \alpha^2 \mathcal{R}_{H_0} \hat{\mathcal{L}}_{\mathcal{R}_{H_0}} \mathcal{R}_{H_0} \hat{\mathcal{R}}_{H_0} + \ldots \]

\[ = \sum_{n=0}^{\infty} (-1)^n \alpha^n \mathcal{R}_{H_0}(z) \left( \hat{\mathcal{L}}_{\mathcal{R}_{H_0}} \mathcal{R}_{H_0}(z) \right)^n. \]

The integration around a small contour results in the Kato series \([11]\) for the “perturbed averaging operator”

\[ \hat{\mathcal{P}}_H = -\frac{1}{2\pi i} \oint_{|z| = \epsilon} \mathcal{R}_H(z)dz = -\frac{1}{2\pi i} \sum_{n=0}^{\infty} \oint_{|z| = \epsilon} (-1)^n \alpha^n \mathcal{R}_{H_0}(z) \left( \hat{\mathcal{L}}_{\mathcal{R}_{H_0}} \mathcal{R}_{H_0}(z) \right)^n dz \]

\[ = -\frac{1}{2\pi i} \sum_{n=0}^{\infty} (-1)^n \alpha^n \oint_{|z| = \epsilon} \left( \sum_{m=0}^{\infty} \mathcal{R}_{H_0}^{(m)} z^m \right) \left( \hat{\mathcal{L}}_{\mathcal{R}_{H_0}} \sum_{k=0}^{\infty} \mathcal{R}_{H_0}^{(k)} z^k \right)^n dz, \]

the “perturbed integrating operator”, and the “perturbed quasi-nilpotent”:

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

Only coefficients of \(z^{-1}\) in these expansions will contribute to the result:

\[ \hat{\mathcal{P}}_H = \sum_{n=0}^{\infty} (-1)^{n+1} \alpha^n \left( \sum_{\sum p_i = n} \mathcal{R}_{H_0}^{(p_1)} \hat{\mathcal{L}}_{\mathcal{R}_{H_0}}^{(p_1)} \cdots \hat{\mathcal{R}}_{H_0}^{(p_1)} \right), \]

\[ \hat{\mathcal{S}}_H = \sum_{n=0}^{\infty} (-1)^n \alpha^n \left( \sum_{\sum p_i = n+1} \mathcal{R}_{H_0}^{(p_1)} \hat{\mathcal{L}}_{\mathcal{R}_{H_0}}^{(p_1)} \cdots \hat{\mathcal{R}}_{H_0}^{(p_1)} \right), \]  

(25)

\[ \hat{\mathcal{D}}_H = \sum_{n=1}^{\infty} (-1)^{n+1} \alpha^n \left( \sum_{\sum p_i = n-1} \mathcal{R}_{H_0}^{(p_1)} \hat{\mathcal{L}}_{\mathcal{R}_{H_0}}^{(p_1)} \cdots \hat{\mathcal{R}}_{H_0}^{(p_1)} \right). \]
A summation in the above expressions should be done by all possible placements of \( n \) (or \( n + 1 \), or \( n - 1 \)) operators \( \dot{S}_H \) in \( n + 1 \) sets. These are also known as a “weak compositions”. There are \( C_{2n}^n \) terms of order \( \alpha^n \) in \( \dot{P}_H \) and \( C_{2n+1}^n \) terms in \( \dot{S}_H \). Here are the first two orders of the “perturbed integrating operator”:

\[
\dot{S}_H = \dot{S} - \alpha(\hat{S}\hat{L}_H \hat{S} - \hat{S}^2 \hat{L}_H \hat{P} - \hat{P}\hat{L}_H \hat{S}^2) + \alpha^2(\hat{S}\hat{L}_H \hat{S}\hat{L}_H \hat{S} - \hat{S}^2 \hat{L}_H \hat{S}\hat{L}_H \hat{P} - \hat{P}\hat{L}_H \hat{S}^2) + O(\alpha^3),
\]

the “perturbed projector”:

\[
\dot{P}_H = \dot{P} - \alpha(\hat{P}\hat{L}_H \hat{S} + \hat{L}_H \hat{P}) + \alpha^2(\hat{P}\hat{L}_H \hat{S}\hat{L}_H \hat{S} + \hat{S}\hat{L}_H \hat{P}\hat{L}_H \hat{S}) + O(\alpha^3)
\]

and, finally, the “perturbed quasi-nilpotent”:

\[
\dot{D}_H = \alpha\hat{P}\hat{L}_H \hat{P} - \alpha^2(\hat{P}\hat{L}_H \hat{P}\hat{L}_H \hat{S} + \hat{P}\hat{L}_H \hat{S}\hat{L}_H \hat{P} + \hat{S}\hat{L}_H \hat{P}\hat{L}_H \hat{P}) + O(\alpha^3).
\]

Properties of unperturbed operators can be extended to their analytic continuations as follows:

\[
\dot{P}_H H = H, \quad \dot{S}_H L_H = 1 - \dot{P}_H, \quad \dot{L}_H \dot{P}_H = \dot{P}_H \dot{L}_H = \dot{D}_H, \text{ etc.}
\]

For details, see Appendix A and the demo “perturbed_operators”.

Quantum mechanical perturbation theory uses series for \( \dot{P}_H \) in order to find the eigenvalues of perturbed Hamiltonian \([2]\). There is no straightforward analogue in classical mechanics. To avoid misunderstanding, it should be noted that \( \dot{P}_H F \) will not be an integral of the perturbed Hamiltonian. This is because \( \dot{L}_H \dot{P}_H = \dot{D}_H \) is nonzero, in general.

Actually, the “perturbed projector” \( \dot{P}_H \) projects onto the analytic continuation of the algebra of integrals of unperturbed Hamiltonian. This does not coincide, in general, with algebra of integrals of perturbed system. In other words, the zero eigenvalue of the Liouville operator may be split by perturbation.

### 4.3. Connection to Poincaré-Lindstedt-Deprit series

To establish a relation between Kato expansion and standard classical perturbation theory, we will demonstrate that the projectors \( \dot{P}_H \) and \( \dot{P}_H \) are connected by canonical transformation. This is the junction point of two very different formalisms.

Indeed, if we construct a transformation

\[
\dot{x} = \exp_D(\alpha \dot{L}_G) x, \quad \dot{H} = \exp_D^{-1}(\alpha \dot{L}_G) H,
\]

connecting the projectors

\[
\dot{P}_H = \exp_D(\alpha \dot{L}_G) \dot{P}_H \exp_D(\alpha \dot{L}_G), \quad (26)
\]
then it follows from $\hat{P}_H H = H$ that the transformed Hamiltonian will be an integral of the unperturbed system

$$
\hat{P}_{H_0} \tilde{H} = \hat{P}_{H_0} \exp^{-1}(\alpha \mathbf{L}_G) H = \exp^{-1}(\alpha \mathbf{L}_G) \hat{P}_H H = \exp^{-1}(\alpha \mathbf{L}_G) H = \tilde{H}.
$$

Therefore, such transformation will directly realize the programme of Poincaré-Lindstedt perturbation theory.

To find the transformation, consider the derivative of the resolvent with respect to the perturbation

$$
\frac{\partial}{\partial \alpha} \mathcal{R}_H(z) = -\mathcal{R}_H(z) \hat{L}_H \mathcal{R}_H(z).
$$

Substitution $z_1 = z_3 = z$ and $F = H_i$ into the canonical resolvent identity \([24]\) results in

$$
\mathcal{R}_H(z) \hat{L}_H \mathcal{R}_H(z) = \hat{L}_H \mathcal{R}_{H(z)} \hat{L}_H \mathcal{R}_H(z) - \mathcal{R}_H(z) \hat{L}_H \mathcal{R}_{H(z)} H_i - z_2 \mathcal{R}_H(z) \hat{L}_H \mathcal{R}_{H(z)} H_i \mathcal{R}_H(z) \tag{27}
$$

Look at the coefficient of $z_0^0$ in the Laurent series of the above expression

$$
\frac{\partial}{\partial \alpha} \mathcal{R}_H(z) = \mathcal{R}_H(z) \hat{L}_H \mathcal{R}_H(z) - \mathcal{R}_H(z) \hat{L}_H \mathcal{R}_H(z) - \mathcal{R}_H(z) \hat{L}_H \mathcal{R}_H(z).
$$

Proceeding the same way for coefficients of $z_2^{-n}$ ($n \geq 1$) in \([27]\), we find

$$
\begin{align*}
\mathcal{R}_H(z) \hat{L}_H \mathcal{R}_H(z) &= \hat{L}_H \mathcal{R}_H(z) - \mathcal{R}_H(z) \hat{L}_H \mathcal{R}_H(z), \\
\mathcal{R}_H(z) \hat{L}_H \mathcal{R}_H(z) &= \hat{L}_H \mathcal{R}_H(z) - \mathcal{R}_H(z) \hat{L}_H \mathcal{R}_H(z).
\end{align*}
$$

This allows for the rewriting of the resolvent derivative as

$$
\frac{\partial}{\partial \alpha} \mathcal{R}_H(z) = \mathcal{R}_H(z) \hat{L}_H \mathcal{R}_H(z) - \mathcal{R}_H(z) \hat{L}_H \mathcal{R}_H(z) - \mathcal{R}_H(z) \hat{L}_H \mathcal{R}_H(z).
$$

Actually, this is a power series because $\hat{D}_H = O(\alpha^n)$.

From the Hilbert identity, it follows that $\frac{\partial^n}{\partial z^n} \mathcal{R}_H(z) = n! \hat{D}_H^{n+1} \mathcal{R}_H(z)$. Finally,

$$
\frac{\partial}{\partial \alpha} \mathcal{R}_H(z) = \mathcal{R}_H(z) \hat{L}_H \mathcal{R}_H(z) - \mathcal{R}_H(z) \hat{L}_H \mathcal{R}_H(z) - \mathcal{R}_H(z) \hat{L}_H \mathcal{R}_H(z)
+ \frac{1}{2} \hat{L}_H \frac{\partial^2 \mathcal{R}_H(z)}{\partial z^2} - \frac{1}{6} \hat{L}_H \frac{\partial^3 \mathcal{R}_H(z)}{\partial z^3} + \ldots \tag{28}
$$

Therefore, change of the resolvent under perturbation $\alpha H_i$ can be represented as a sum of canonical transformation with generator $-\hat{S}_H H_i$ and resolvent transformation as a function of complex variable $z$.

The derivative of projector $\frac{\partial}{\partial \alpha} \hat{P}_H$ may be obtained as the residue of the previous expression at $z = 0$. In our case of isolated point spectrum, the resolvent is a
meromorphic function, and the residue of any its derivative with respect to \( z \) vanishes. Therefore, the projector \( \hat{P}_H \) transforms canonically under perturbation

\[
\frac{\partial}{\partial \alpha} \hat{P}_H = \hat{P}_H \hat{L}_{S_H H_i} - \hat{L}_{S_H H_i} \hat{P}_H, \tag{29}
\]

and the projectors are connected by the Lie transform with generator \( -\hat{S}_H H_i \):

\[
\hat{P}_H = \exp_D(\alpha \hat{L}_{-S_H H_i}) \hat{P}_{H_0} \exp_D^{-1}(\alpha \hat{L}_{-S_H H_i}).
\]

We see that the canonical transformation with generator

\[
G = -\hat{S}_H H_i = \sum_{n=0}^{\infty} (-1)^{n+1} \alpha^n \left( \sum_{\sum p_i = n+1 \atop p_i \geq 0} \hat{R}_{H_0}^{(p_{n+1})} \hat{L}_{H_i} \hat{R}_{H_0}^{(p_n)} \hat{R}_{H_0}^{(p_2)} \hat{L}_{H_i} \hat{R}_{H_0}^{(p_1)} H_i \right), \tag{30}
\]

formally normalizes the Hamiltonian in all orders in \( \alpha \).

4.4. General form of generator.

Knowing that \( \hat{P}_{H_0} \) and \( \hat{P}_H \) are canonically connected and that this transformation normalizes the Hamiltonian, we can reformulate the programme of Poincaré-Lindstedt perturbation theory to the construction of canonical transformation, which connects unperturbed and perturbed averaging operators.

Let us now determine the general form of such a transformation. It follows from \cite{26} that \( \hat{P}_H \) satisfies the operatorial differential equation

\[
\frac{\partial}{\partial \alpha} \hat{P}_H = \hat{L}_G \hat{P}_H - \hat{P}_H \hat{L}_G.
\]

Application of this expression to Hamiltonian \( H \) results in

\[
\left( \frac{\partial}{\partial \alpha} \hat{P}_H \right) H = \hat{L}_G \hat{P}_H H - \hat{P}_H \hat{L}_G H.
\]

Since \( \hat{P}_H H = H \), \( \frac{\partial}{\partial \alpha} (\hat{P}_H H) = \left( \frac{\partial}{\partial \alpha} \hat{P}_H \right) H + \hat{P}_H \frac{\partial H}{\partial \alpha} \) and \( \frac{\partial H}{\partial \alpha} = H_i \), the previous expression becomes

\[
(1 - \hat{P}_H) \hat{L}_H G = -(1 - \hat{P}_H) H_i.
\]

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

\[
G = -\hat{S}_H H_i + \hat{P}_H F, \tag{31}
\]

where \( F(x) \) may be any analytic function. This is the central formula of this work. It provides a non-recursive expression for the generator of Poincaré-Lindstedt transformation and defines its ambiguity.
The choice of function $F$ is the normalization style. It is natural to choose $F(x) \equiv 0$ or $\mathbf{P}_H G = 0$. This is not equal to the “non-secular” normalization $\mathbf{P}_{H_0} G_D = 0$ traditionally used for Deprit generator in classical perturbation theory. Because $\mathbf{L}_F \mathbf{P}_H = \mathbf{P}_H \mathbf{L}_F$, the projector $\mathbf{P}_H$ itself is not sensitive to normalization style.

We may conclude that the generators of normalizing transformations may differ by a function belonging to a continuation of algebra of integrals of unperturbed system. Illustration can be found in the demo “styles” in the Supplementary data files.

Quantum mechanical Kato perturbation expansion uses another formulae for unitary transformation connecting the unperturbed and perturbed projectors \[11\]. However, the original Kato generator and the rational expression developed by Szőkefalvi-Nagy \[11\] do not define canonical transformations in classical mechanics.

4.5. The first orders.

Let us compare the expressions for generator

\[
G = -\hat{S} H_i + \alpha \left( \hat{S} \hat{L} \hat{S} H_i - \hat{S}^2 \hat{L} \hat{P} H_i \right) - \alpha^2 \left( \hat{S} \hat{L} \hat{S} \hat{L} \hat{S} H_i - \hat{S} \hat{L} \hat{S}^2 \hat{L} \hat{P} H_i \right)
\]

\[
- \hat{S}^2 \hat{L} \hat{S} \hat{L} \hat{P} H_i - \hat{S}^2 \hat{L} \hat{P} \hat{L} \hat{S} H_i - \hat{P} \hat{L} \hat{S} \hat{L} \hat{S}^2 H_i - \hat{P} \hat{L} \hat{S} \hat{L} \hat{S} \hat{L} \hat{S} H_i
\]

\[
+ \hat{S}^3 \hat{L} \hat{P} \hat{L} \hat{P} H_i + \hat{P} \hat{L} \hat{S} \hat{L} \hat{P} H_i + \hat{P} \hat{L} \hat{P} \hat{L} \hat{S}^3 H_i + O(\alpha^3), \tag{32}
\]

and normalized Hamiltonian

\[
\hat{H} = H_0 + \alpha \hat{P} H_i - \frac{\alpha^2}{2} \hat{P} \hat{L} \hat{S} H_i + \alpha^3 \left( \frac{1}{3} \hat{P} \hat{L} \hat{S} \hat{L} \hat{S} H_i - \frac{1}{6} \hat{P} \hat{L} \hat{S}^2 \hat{L} \hat{P} H_i \right) + \alpha^4 \left( \frac{1}{6} \hat{P} \hat{L} \hat{S} \hat{L} \hat{S} \hat{L} \hat{P} H_i \right)
\]

\[
- \frac{1}{4} \hat{P} \hat{L} \hat{L} \hat{S} \hat{L} \hat{S} \hat{L} \hat{S} H_i + \frac{1}{12} \hat{P} \hat{L} \hat{S} \hat{L} \hat{S} \hat{L} \hat{S} \hat{L} \hat{P} H_i + \frac{1}{8} \hat{P} \hat{L} \hat{S} \hat{L} \hat{P} \hat{L} \hat{S} \hat{L} \hat{S} H_i + \frac{1}{4} \hat{P} \hat{L} \hat{P} \hat{L} \hat{S} \hat{L} \hat{S} \hat{L} \hat{S} H_i
\]

\[
+ \frac{1}{4} \hat{P} \hat{L} \hat{P} \hat{L} \hat{S} \hat{L} \hat{S} \hat{L} \hat{P} H_i - \frac{1}{6} \hat{P} \hat{L} \hat{P} \hat{L} \hat{S} \hat{L} \hat{P} \hat{L} \hat{S}^3 H_i + O(\alpha^5) \tag{33}
\]

with the Deprit series \[16\]. Here we have denoted $\mathbf{L} = \mathbf{L}_{H_i}$ for compactness and used the identities $\mathbf{P}_L \hat{S} \hat{L} \mathbf{S} \hat{H}_i \equiv 0$ and $\mathbf{P}_L \hat{P} \hat{H}_i \equiv 0$.

At these orders, series \[16\] and \[33\] are very close and differ only by secular terms in the generator. This is because of the natural normalization style $\mathbf{P}_H G = 0$. In higher orders, the differences also propagate in non-secular terms. Due to these additional terms, our expressions for the generator and normalized Hamiltonian become linear and systematic. Actually, because of canonical identities, there are many equivalent expressions for generator and Hamiltonian. In next section we will develop another explicitly secular one.

Larger formula for the Hamiltonian normalized up to $O(\alpha^8)$ can be found in the demo “normalized_hamiltonian7” in the supplementary data files. It consist of 528 terms and the corresponding generator has 2353 terms.
Example 1. Duffing equation. This is one-dimensional oscillator with the quartic anharmonicity:

\[ H = \frac{1}{2}(p^2 + q^2) + \frac{\alpha}{4}q^4 = J + \alpha J^2 \cos^4(\phi). \]

The following are Birkhoff and “Action-Angle” representations of normalizing generator:

\[
G = \frac{pq}{32} (3p^2 + 5q^2) - \alpha \frac{pq}{384} (39p^4 + 104p^2q^2 + 57q^4) + O(\alpha^2)
\]

\[
= -\frac{J^2}{32} \left(8 \sin(2\phi) + \sin(4\phi)\right) + \frac{\alpha J^3}{192} \left(99 \sin(2\phi) + 9 \sin(4\phi) - \sin(6\phi)\right) + O(\alpha^2)
\]

The normalized Hamiltonian is as follows:

\[
\tilde{H} = \frac{1}{2}(p^2 + q^2) + \frac{3\alpha}{32} (p^2 + q^2)^2 - \frac{17\alpha^2}{512} (p^2 + q^2)^3 + \frac{375\alpha^3}{16384} (p^2 + q^2)^4 + O(\alpha^4)
\]

\[
= J + \frac{3}{8} \alpha J^2 - \frac{17}{64} \alpha^2 J^3 + \frac{375}{1024} \alpha^3 J^4 + O(\alpha^4).
\]

This is the typical structure of the perturbation series for nonresonant systems. More terms can be found in the demo “anharmonic”. Because of the uniqueness of the nonresonant normal form \[18\], the normalized Hamiltonian coincides with the classical Deprit series.

5. Multidimensional systems.

5.1. Truncated series.

An extension of the previous construction to the multidimensional case causes difficulty. The spectrum of the Liouville operator for multi-frequency dynamical system is a union of countably many additive groups \[12\]. Typically, singularities of the multidimensional resolvent cannot be separated from the origin. This is the classic problem of small denominators. The resolvent is no more holomorphic \[15\] and we can therefore no longer directly rely on Kato series \[25\] and residues.

But our computer algebra calculations confirm the validity of the expression \[30\] for generator in the first orders of multidimensional case also. The key point here is the canonical connection between perturbed and unperturbed projectors. Using the demo “phdot”, we checked it by brute force computation up to \(\alpha^{10}\). The simplification of almost three million terms took a week of computer time.

Therefore, we can suggest that formula \[30\] remains (asymptotically) valid. But more proof is needed that uses the canonical identities \[11 - 14\] and does not rely on the resolvent and spectrum of Liouville operator.

In the Appendices, we present this alternate proof. It follows the ideas of the previous sections, but uses truncated at order \(N\) finite operatorial sums. Appendix A discusses the properties of truncated operators \(\hat{P}_H^{[N]}\), \(\hat{S}_H^{[N]}\) and \(\hat{D}_H^{[N]}\), and in Appendix B we demonstrate that for any \(N \in \mathbb{N}, N \geq 2\), the perturbed truncated projector...
transforms canonically:

\[
\left( \frac{\partial}{\partial \alpha} \mathcal{P}_H \right)^{[N]} = \mathcal{L}_{-S_H^{[N]} H_i} \mathcal{P}_H^{[N]} - \mathcal{P}_H^{[N]} \mathcal{L}_{-S_H^{[N]} H_i} + O(\alpha^{N+1}). \tag{35}
\]

Combining this with the Lie transform, we can conclude that the transformation with generator \( G^{[N]} = -S_H^{[N]} H_i \) normalizes Hamiltonian to the order \( N \):

\[
\tilde{H}^{[N]} = \exp_D^{-1}(\alpha \hat{L}_{-S_H^{[N]} H_i}) H + O(\alpha^{N+1}) = \exp_D^{-1}(\alpha \hat{L}_{-S_H^{[N]} H_i}) \hat{P}_H^{[N]} H + O(\alpha^{N+1})
\]

\[
= \hat{P}_{H_0} \exp_D^{-1}(\alpha \hat{L}_{-S_H^{[N]} H_i}) H + O(\alpha^{N+1}) = \hat{P}_{H_0} \tilde{H}^{[N]} + O(\alpha^{N+1}).
\]

This establishes formally asymptotic character of series.

The small denominators also affect the unperturbed operators \( \hat{P}_{H_0} \) and \( \hat{S}_{H_0} \) defined by (8). This classical problem was first encountered in celestial mechanics by H. Bruns in 1884. Fundamental works of Kolmogorov [13] and Arnold [44] thoroughly investigated the analytical properties of averaging operation and the solution of homological equation. For general non-degenerate multidimensional system these operators are analytic for all frequencies, except for a set of Lebesgue measure zero. This is sufficient for our formal constructions. It is worth mentioning that the problem does not concern applications in which perturbation is represented by finite Fourier sums.

### 5.2. Non-uniqueness of the normalized Hamiltonian.

Similarly to (31), the general form of the truncated generator of the Poincaré-Lindstedt transformation is

\[
G^{[N]} = -S_H^{[N]} H_i + \hat{P}_H^{[N]} F,
\]

where \( F(x) \) defines the normalization style. Now it is possible to discuss its effects.

For the sake of clarity, we will hereafter use formal “analytic” expressions, as in the previous chapters. However, one must always remember that for mathematical correctness, these expressions must be straightforwardly converted into truncated sums (up to \( O(\alpha^{N+1}) \)).

Following Koseleff [18], consider two Hamiltonians normalized in different styles:

\[
\tilde{H}_1 = \exp_D^{-1}(\alpha \hat{L}_{G_1}) H \quad \text{and} \quad \tilde{H}_2 = \exp_D^{-1}(\alpha \hat{L}_{G_2}) H.
\]

These quantities are connected by the transformation

\[
\tilde{H}_2 = \exp_D^{-1}(\alpha \hat{L}_{G_2}) \exp_D(\alpha \hat{L}_{G_1}) \tilde{H}_1 = \hat{U}_{21} \tilde{H}_1.
\]

Obviously, \( \hat{U}_{21} \) is canonical. Let us find its generator. By derivation, we obtain

\[
\frac{\partial}{\partial \alpha} \hat{U}_{21} = \exp_D^{-1}(\alpha \hat{L}_{G_2}) \left( \hat{L}_{G_1} - \hat{L}_{G_2} \right) \exp_D(\alpha \hat{L}_{G_1}) = \exp_D^{-1}(\alpha \hat{L}_{G_2}) \hat{L}_{G_1 - G_2} \exp_D(\alpha \hat{L}_{G_1})
\]

\[
= \exp_D^{-1}(\alpha \hat{L}_{G_2}) \hat{L}_{P_H F_2} \exp_D(\alpha \hat{L}_{G_1}) = \hat{L}_{\exp_D^{-1}(\alpha \hat{L}_{G_2}) P_H F_2} \hat{U}_{21}.
\]

Due to (31), the difference of the generators always has the form \( \hat{P}_H F_2 \) with some function \( F_2(x) \). Because of (20), the generator of \( \hat{U}_{21} \) is secular

\[
G_{21} = \exp_D^{-1}(\alpha \hat{L}_{G_2}) \hat{P}_H F_2 = \hat{P}_{H_0} \exp_D^{-1}(\alpha \hat{L}_{G_2}) F_{21}.
\]
We may conclude that the normalized Hamiltonians are connected by the Lie transform, with the generator belonging to the algebra of integrals of unperturbed system.

For non-resonance system with incommensurable frequencies, all these integrals are commutative. As a consequence, non-resonance normal form is unique and insensitive to normalization style \[18\].

This is not so in the case of resonance. Because resonance relations give rise to non-commutative integrals, the normalized resonance Hamiltonian depends on the style.

We can obtain expression for $\tilde{H}$ following idea of Vittot \[45\]. Consider the derivative

$$
\frac{\partial}{\partial \alpha} \tilde{H} = \left( \frac{\partial}{\partial \alpha} \exp_D^{-1}(\alpha \hat{L}_G) \right) H + \exp_D^{-1}(\alpha \hat{L}_G) \frac{\partial}{\partial \alpha} H = \exp_D^{-1}(\alpha \hat{L}_G) \left( \hat{L}_H G + H_i \right)
$$

$$
= \exp_D^{-1}(\alpha \hat{L}_H, H_i + \hat{D}_HF) = \hat{P}_H \exp_D^{-1}(\alpha \hat{L}_H, H_i + \hat{D}_HF) (H_i + \hat{D}_HF).
$$

Here we use \[2\] and the canonical connection of the projectors \[26\]. Therefore,

$$
\tilde{H} = H_0 + \hat{P}_H \int_0^\alpha \exp_D^{-1}(\epsilon \hat{L}_H, H_i + \hat{D}_HF) (H_i + \hat{D}_HF) d\epsilon.
$$

This expression demonstrates the explicit dependence on $F(x)$.

5.3. Gustavson integrals

It is of interest to find physically meaningful quantities that are insensitive to an artificial choice of normalization style $F(x)$. Consider a system with constant unperturbed frequencies. In his celebrated article Gustavson \[28\] constructed the formal integrals for a perturbed system originating from the centre of algebra of integrals of unperturbed system.

More precisely, each resonance relation for unperturbed frequencies $(\vec{\omega}, \vec{D}_k) = 0$, $k = 1, \ldots, r$ results in an additional non-commutative integral. In Birkhoff and “Action-Angle” representations, the centre of corresponding algebra of integrals consist of the $d - r$ quantities

$$
\tilde{I}_i = \sum_{j=1}^d \beta_{ij} \tilde{\zeta}_j \tilde{\eta}_j = (\tilde{\beta}_i, \tilde{J}), \quad i = 1, d - r.
$$

Here, $\tilde{\beta}_i$ is a set of $d - r$ independent vectors orthogonal to all $r$ resonance vectors $\vec{D}_k \ [28]$.

These integrals are commutative with all integrals of the unperturbed system, and therefore with normalized Hamiltonian $\tilde{H}$. In operator notation, for any analytic $\tilde{F}(x)$,

$$
\tilde{I}_i = \hat{P}_H \tilde{I}_i, \quad i = 1, d - r,
$$

$$
[\tilde{I}_i, \hat{P}_H \tilde{F}] = 0,
$$

$$
[\tilde{I}_i, \tilde{H}] = 0.
$$

After the transformation back to the initial variables, the quantities

$$
I_i = \exp_D(\alpha \hat{L}_G) \tilde{I}_i, \quad i = 1, d - r,
$$

(37)
become formal integrals of the perturbed system. Moreover, these Gustavson integrals are commutative with all functions in the image of $\hat{\mathbf{P}}_{H}$:

$$I_i = \exp_D(\alpha \mathbf{L}_G) \hat{\mathbf{P}}_{H_0} \tilde{I}_i = \hat{\mathbf{P}}_{H} \exp_D(\alpha \mathbf{L}_G) \tilde{I}_i = \hat{\mathbf{P}}_{H} I_i, \quad i = 1, d - r,$$

$$[I_i, \hat{\mathbf{P}}_{H} F] = \exp_D(\alpha \mathbf{L}_G) [\tilde{I}_i, \hat{\mathbf{P}}_{H_0} \exp_D^{-1}(\alpha \mathbf{L}_G) F] = 0,$$

$$[I_i, H] = \exp_D(\alpha \mathbf{L}_G) [\tilde{I}_i, \tilde{H}] = 0.$$

Here we have again used the canonical connection of the projectors \[26\]. Due to the above properties, the derivative of $I_i(\alpha)$ will not depend on $F(x)$:

$$\left( \frac{\partial}{\partial \alpha} I_i(\alpha) \right) = \left( \frac{\partial}{\partial \alpha} \exp_D(\alpha \mathbf{L}_G) \right) \tilde{I}_i = \mathbf{L}_G I_i = -\mathbf{L}_{\mathbf{S}_H H_i} I_i + \mathbf{L}_{\mathbf{P}_H} I_i = -\mathbf{L}_{\mathbf{S}_H H_i} I_i.$$

Therefore, Gustavson integrals $I_i(\alpha)$ are insensitive to normalization style. Actually, these quantities diverge \[10\], but are useful in exploring the regions of regular dynamics.

The unperturbed Hamiltonian $H_0$ itself may be chosen as a seed for $\tilde{I}_i$. First orders of the nontrivial part of the corresponding Gustavson integral are

$$I_G = \alpha^{-1} \left( H - \exp_D(\alpha \mathbf{L}_{-\mathbf{S}_H H_i}) H_0 \right) = \hat{\mathbf{P}}_{H_i} - \alpha \left( \mathbf{S}_L \hat{\mathbf{P}}_{H_i} + \frac{1}{2} \mathbf{P}_L \mathbf{S}_H I_i \right)$$

$$+ \alpha^2 \left( \mathbf{S}_L \mathbf{S}_L \mathbf{P}_{H_i} + \frac{1}{2} \mathbf{S}_L \mathbf{P}_L \mathbf{S}_H I_i + \frac{1}{3} \mathbf{P}_L \mathbf{S}_L \mathbf{S}_H I_i - \frac{2}{3} \mathbf{P}_L \mathbf{S}_L^2 \mathbf{P}_{H_i} - \frac{1}{3} \mathbf{P}_L \mathbf{P}_L \mathbf{S}_L^2 I_i \right) + \mathcal{O}(\alpha^3).$$

This series is also applicable to general system with non-constant unperturbed frequencies. See the demo “Gustavson_integral”. It is known as the Hori’s formal first integral \[19\].

**Example 2. Hénon-Heiles system.** This is a two-dimensional system with Hamiltonian

$$H = \frac{1}{2} (p_1^2 + q_1^2 + p_2^2 + q_2^2) + \alpha (q_1^3 q_2 - \frac{1}{3} q_2^3).$$

In complex $\zeta, \eta$ variables \[71\] the Hénon-Heiles Hamiltonian becomes

$$H = i \zeta_2 \eta_2 + i \zeta_1 \eta_1 + \alpha \frac{1}{2 \sqrt{2}} \left( \zeta_2 \eta_2^3 - \frac{1}{3} \zeta_2^3 - \eta_1^2 \zeta_2 - 2 \zeta_1 \eta_1 \eta_2 + \zeta_2^2 \zeta_2^2 \right)$$

$$+ \frac{1}{3} i \eta_2^3 - i \zeta_2^2 \eta_2 - i \eta_1^2 \eta_2 - 2 i \zeta_1 \eta_1 \zeta_2 + i \zeta_1^2 \eta_2).$$

The first orders of the normal form are

$$\tilde{H} = i \left( \zeta_2 \eta_2 + i \zeta_1 \eta_1 \right) + \alpha^2 \left( \frac{5}{12} \zeta_2^2 \eta_2^2 + \frac{7}{12} \eta_1 \zeta_2 \eta_2 - \frac{1}{3} \zeta_1 \eta_1 \zeta_2 \eta_2 + \frac{7}{12} \zeta_1^2 \eta_2^2 + \frac{5}{12} \zeta_1^2 \eta_1 \right)$$

$$+ i \alpha^4 \left( \frac{235}{32} \zeta_2^3 \eta_2^3 - \frac{175}{144} \zeta_2^2 \eta_2^3 \eta_2^3 - \frac{47}{16} \zeta_1 \eta_1 \zeta_2 \eta_2^2 + \frac{161}{144} \zeta_1 \eta_1^3 \zeta_2 \right)$$

$$- \frac{175}{144} \zeta_1 \eta_2^2 + \frac{65}{16} \zeta_1^2 \eta_2^2 \zeta_2 + \frac{161}{144} \zeta_1 \eta_1 \zeta_2^2 \eta_2 - \frac{101}{16} \zeta_1 \eta_1^3 \eta_2^2 + \mathcal{O}(\alpha^6).$$

Because this is the $1 : 1$ resonance system, we see here mixed terms, such as $\zeta_1 \eta_2$. First orders of the Gustavson integral are

$$I_G = \alpha^{-2} (H - \exp_D(\alpha \mathbf{L}_G) H_0) = -\frac{1}{45} \left( 5 p_1^4 + 2 p_2^4 (5 p_2^2 + 5 q_2^2 - 9 q_3^2) + 56 p_1 p_2 q_1 q_2 + 5 p_2^4 \right)$$

$$- 2 p_2^2 (9 q_1^2 - 5 q_2^2) + 5 \left( q_1^2 + q_2^2 \right)^2 \right) - \alpha \frac{1}{36} \left( -28 p_1^4 q_2 + 28 p_1^2 p_2 q_1 + p_1^2 q_2 (84 p_2^2 - 27 q_1^2 + 37 q_2^2) \right.$$

$$+ 42 p_1 p_2 q_1 \left( -2 p_2^2 + q_1^2 + q_2^3 \right) - p_2^2 (69 q_1^2 q_2 + 5 q_2^3) - 5 q_2 \left( q_2 - 3 q_1^2 \left( q_1^2 + q_2^2 \right) \right) + \mathcal{O}(\alpha^2)$$

\[22\]}
In these orders, the expressions are identical to those of classical works [28, 47]. Further orders can be found in the demo “Henon-Heiles”. The differences between these and the Deprit series begin at fifth order in generators and the eighth order in the normalized Hamiltonians.

As expected, the difference between generators belongs to the kernel of $1 - \hat{P}_H$ and the normalized Hamiltonians are connected by the Lie transform with the secular generator. The Gustavson integrals are identical up to the highest order that we computed.

It is now necessary to say several words about nonresonant systems. The KAM theory [44, 48] showed that nonresonant dynamical systems are stable against small perturbations in the sense that a majority of its invariant tori will not destruct. Works of Elliasson, Gallavotti and others [49, 50] demonstrated the convergence of Poincaré-Lindstedt series on nonresonant set and the systematic cancellations of small denominators. It is natural to search for nonresonance cancellations in Kato series too. Such cancellations, connections to Whittaker’s adelphic integrals and corresponding computational algorithms will be discussed in separate article.

### 6. Computational aspects.

A major difference between this and classical perturbation algorithms by Deprit [4], Hori [19], Dragt and Finn [5], etc. is the explicit non-recursive formulae. Traditionally, perturbation computations solve homological equations order by order. In contrast, we directly compute generator $G = -\hat{S}_H H_i$ up to the desired order as a sum of all permutations (30). This is reminiscent of diagrammatic expansions in quantum field theory. Then, Lie transform normalizes the Hamiltonian. We present the details of the explicit “Square” algorithm for the generator in Appendix C.

The explicit expressions are important from a general mathematical point of view, as they systematize and simplify the perturbation expansion, at the price of additional secular terms in the generator. Due to these terms, our approach will be less effective for the practical computations than the classical Deprit algorithm. However, this should not be a serious problem for contemporary computers.

We compared the computational times of the direct normalization $\tilde{H} = \exp_D^{-1}(\alpha L -\hat{S}_H H_i) H$ using the explicit expression (30) with those of the Deprit algorithm [4] and the algorithm of Dragt and Finn [5]. The latter method uses the products of canonical transformations

$$\tilde{x} = e^{\alpha L_{G_0}} \ldots e^{\alpha L_{G_{n-1}}} x,$$

instead of Lie transforms (Deprit exponents) in order to normalize Hamiltonian.

Table 1 compares the times for computing the normal form for the one-dimensional anharmonic oscillator and the two-dimensional Hénon-Heiles system on an Intel Xeon X5675 (3.06 GHz) processor.
Table 1. Normalization time (s).

| Order | Anharmonic (1d) | Hénon-Heiles (2d) |
|-------|-----------------|-------------------|
|       | Deprit          | Dragt & Finn      | Explicit | Deprit | Dragt & Finn | Explicit |
| 4     | 0.02 0.01 0.04  | 0.05 0.04 0.1     |
| 8     | 0.12 0.06 0.3   | 0.5 1.2 1.3    |
| 16    | 1.7 0.8 6.     | 19. 139. 42.   |
| 24    | 10.7 3.5 49.   | 345. 2231. 558. |
| 32    | 46.1 10.2 235. | 3155. 20930. 432. |

The table reveals that our method is indeed slower than Deprit, but is still fast enough to complete practical computations. Dragt and Finn’s method is faster for one-dimensional systems and lower orders, but is less effective for computing higher orders. This is a consequence of the growing number of exponentiations intrinsic to it. The number of the Poisson bracket evaluation in Dragt and Finns method is smaller than that of in Deprits algorithm [1], but the brackets have larger arguments.

All the methods build near-identity normalizing canonical transformations. Such transformations are always the Hamiltonian flows equivalent to Deprit transformation with different normalization styles \( \mathbf{P}_H F \). As expected, all three normal forms differ from each other starting from the 8th order, while the series for Gustavson integrals coincide. It is the advantage of explicit formula (30) that we are able to compute Gustavson integrals without the previous normalization.

It is worth noting that the above computations were single-threaded. If needed, the sum of all the placements in (30) can be parallelized and made scalable for contemporary multi-CPU and Cloud computing.

7. Beyond the perturbation expansion.

Because we now have the explicit expression for the generator of the Poincaré-Lindstedt transformation, it is interesting to apply it to determine an exact solution and construct an explicit expression for \( \mathbf{S}_H H_i \). This is possible only for trivial systems because it requires algebraic integrability for all \( \alpha \). However, the following toy examples nicely illustrate the perturbation expansion:

Example 3. Shift of frequency of the harmonic oscillator.

\[
H = \frac{1}{2}(p^2 + q^2) + \frac{\alpha}{2} q^2.
\]

Here we know the exact solution, \( q(t) = \sqrt{\frac{2E}{1+\alpha}} \cos(\sqrt{1+\alpha}t + \phi) \), where the constant energy \( E = H(p, q) \) and \( \phi \) are the functions of the initial point \( (p_0, q_0) \).

We can directly calculate the “exact” perturbation operators using (17) and then
substitute \( p_0 \rightarrow p \), \( q_0 \rightarrow q \) as follows:

\[
\frac{\hat{\mathbf{P}}}{2} \frac{q^2}{2} = \lim_{\lambda \to +0} \lambda \int_{0}^{+\infty} e^{-\lambda t} q(t)^2 dt = \frac{H}{2(1 + \alpha)},
\]

\[
\frac{\hat{\mathbf{S}}}{2} \frac{q^2}{2} = -\lim_{\lambda \to +0} \lambda \int_{0}^{+\infty} e^{-\lambda t} \left( \frac{q(t)^2}{2} - \frac{\hat{\mathbf{P}} H}{2} \right) dt = -\frac{pq}{4(1 + \alpha)}.
\]

Indeed,

\[
\hat{\mathbf{L}}_{\mathcal{H}} \left( -\frac{pq}{4(1 + \alpha)} \right) = -\frac{p^2 + q^2(1 + \alpha)}{4(1 + \alpha)} = \frac{q^2}{2} - \hat{\mathbf{P}} \frac{q^2}{2}.
\]

Therefore, the exact generator is \( G = \frac{pq}{4(1 + \alpha)} \). The normalizing canonical transformation ("Deprit exponent") is determined by the equations

\[
\frac{\partial p}{\partial \alpha} = \hat{\mathbf{L}}_G p = -\frac{p}{4(1 + \alpha)},
\]

\[
\frac{\partial q}{\partial \alpha} = \hat{\mathbf{L}}_G q = \frac{q}{4(1 + \alpha)},
\]

with the straightforward solution

\[
\tilde{p} = \frac{1}{\sqrt{1 + \alpha}} p, \quad \tilde{q} = \sqrt{1 + \alpha} q.
\]

The normalized Hamiltonian is \( \tilde{H} = \sqrt{1 + \alpha} (\frac{p^2}{2} + \frac{q^4}{4}) \). The power series for these exact generator and Hamiltonian coincide with the standard perturbation expansion.

**Example 4. The Duffing equation. Part II.**

\[
H = \frac{1}{2} \left( \frac{p^2}{2} + \frac{q^2}{2} \right) + \frac{\alpha}{4} q^4.
\]

This system allows for an exact solution using Jacobi elliptic functions:

\[
q(t) = A \cn(\omega t + \psi, k^2),
\]

\[
\omega^2 = \sqrt{1 + 4\alpha E}, \quad A^2 = \frac{1}{\alpha} (\omega^2 - 1), \quad k^2 = \frac{1}{2} (1 - \frac{1}{\omega^2}).
\]

Here, the energy \( E = H(p_0, q_0) \) and "pseudo-phase" \( \psi \) are determined by the initial condition

\[
\frac{\sn(\psi, k^2)}{\cn(\psi, k^2)} \dn(\psi, k^2) = -\frac{p_0}{q_0 \omega}.
\]

In order to find the exact integrating operator \( \hat{\mathbf{S}} H_i \), we may expand the perturbation \( H_i = \frac{1}{4} q^4 \) into a Fourier series using \[51\]

\[
\cn^4(u, k^2) = \text{const} + \frac{4\pi^2}{3k^4 K^2} \sum_{n=1}^{\infty} \frac{n Q^n}{1 - Q^{2^n}} \left( (2k^2 - 1) + \frac{n^2 \pi^2}{4K^2} \right) \cos \left( \frac{n\pi}{K} u \right).
\]

Here, \( K(k^2) \) is the complete elliptic integral of the first kind, and

\[
Q = \exp \left( -\frac{\pi K(k^2)}{K(1 - k^2)} \right).
\]
is the “elliptic nome”.

The normalizing generator will be

\[ G = -\hat{S}_H H_i = \lim_{\lambda \to +0} \int_0^\infty e^{-\lambda t} \left( \frac{q(t)^4}{4} - \hat{P}_H H_i \right) dt \]

\[ = -\frac{\pi A^4}{3k^4\omega K} \sum_{n=1}^\infty \frac{Q^n}{1 - Q^{2n}} \left( \frac{n^2 \pi^2}{4K^2} - \frac{1}{\omega^2} \right) \sin \left( \frac{n\pi}{K} \psi \right). \] (39)

For comparison with standard perturbation expansion, we introduce the \(2\pi\)-periodic “pseudo-phase” \(\theta = \frac{\pi}{2K} \psi\). This angle can be obtained from (38) as a power series (again, we substituted \(p_0 \to p, q_0 \to q\)):

\[ \tan(\theta) = -\frac{p}{q} + \frac{p(3p^2 + 5q^2)}{4q(p^2 + q^2)} k^2 + O(k^4). \]

Now we can expand the exact formula (39) into a power series with the help of Wolfram Mathematica®:

\[ G = \frac{pq}{32} (3p^2 + 5q^2) - \alpha \frac{pq}{384} (39p^4 + 104p^2q^2 + 57q^4) + O(\alpha^2). \]

This coincides with perturbation series (31). Surprisingly, the expansion consumes much more computer time than do perturbative computations.

8. Summary.

Being inspired by the deep parallelism between quantum and classical perturbation theories, we have applied Kato resolvent perturbation expansion to classical mechanics. Invariant definitions of averaging and integrating operators and canonical identities uncovered the regular pattern of perturbation series. This pattern was explained using the relation of perturbation operators to the Laurent coefficients of Liouville operator resolvent.

The Kato series for perturbed resolvent and the resolvent canonical identity systematize the perturbation expansion and lead to new explicit expression for the Deprit generator of Poincare-Lindstedt transformation in any order:

\[ G = -\hat{S}_H H_i. \]

Here, the integrating operator \(\hat{S}_H\) is the partial pseudo-inverse of the perturbed Liouville operator. We have used non-perturbative examples to illustrate this formula.

After extending the formalism to multidimensional systems, we described ambiguities of generator and normalized Hamiltonian. Interestingly, Gustavson integrals turn out to be insensitive to normalization style.

All our discussion has remained at a formal level. A comparison of computational times for this approach and for classic Deprit and Dragt&Finn algorithms demonstrated that our series is reasonably efficient even for high orders of perturbation expansion.
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Appendix A. Properties of perturbed operators.

Let us explore the properties of truncated perturbed operators $\hat{P}_H^{[N]}$, $\hat{S}_H^{[N]}$ and $\hat{D}_H^{[N]}$:

$$
\hat{P}_H^{[N]} = \sum_{n=0}^{N} (-1)^{n+1} \alpha^n \left( \sum_{\sum p_i = n} \hat{R}_{H_0}^{(p_{n+1})} \hat{L}_{H_1} \hat{R}_{H_0}^{(p_n)} \cdots \hat{R}_{H_0}^{(p_2)} \hat{L}_{H_0} \hat{R}_{H_0}^{(p_1)} \right),
$$

$$
\hat{S}_H^{[N]} = \sum_{n=0}^{N} (-1)^{n} \alpha^n \left( \sum_{\sum p_i = n+1} \hat{R}_{H_0}^{(p_{n+1})} \hat{L}_{H_1} \hat{R}_{H_0}^{(p_n)} \cdots \hat{R}_{H_0}^{(p_2)} \hat{L}_{H_0} \hat{R}_{H_0}^{(p_1)} \right),
$$

$$
\hat{D}_H^{[N]} = \sum_{n=1}^{N} (-1)^{n+1} \alpha^n \left( \sum_{\sum p_i = n-1} \hat{R}_{H_0}^{(p_{n+1})} \hat{L}_{H_1} \hat{R}_{H_0}^{(p_n)} \cdots \hat{R}_{H_0}^{(p_2)} \hat{L}_{H_0} \hat{R}_{H_0}^{(p_1)} \right).
$$

Here, $[N]$ is the index. We will assume that $N \geq 2$. It is useful to introduce operators

$$
\hat{Z}^m_n = \begin{cases} 
(-1)^{n+1} \sum_{p_1 + \cdots + p_{n+1} = m} \hat{R}_{H_0}^{(p_{n+1})} \hat{L}_{H_1} \hat{R}_{H_0}^{(p_n)} \cdots \hat{R}_{H_0}^{(p_2)} \hat{L}_{H_0} \hat{R}_{H_0}^{(p_1)} & \text{if } m \geq 0, \\
0 & \text{if } m < 0.
\end{cases}
$$

(A.1)

The summation runs over all possible placements of $m$ operators $\hat{S}_{H_0}$ in $n + 1$ sets.

It is important that $\hat{Z}$ operators can be computed recursively. For any $k, 0 \leq k \leq n - 1$

$$
\hat{Z}^m_n = \sum_{i=0}^{m} \hat{Z}^{m-i}_{n-k-1} \hat{L}_{H_1} \hat{Z}^{i}_k.
$$

(A.2)

The simplest such operators are $\hat{Z}^0_0 = \hat{P}$, and $\hat{Z}^m_0 = -\hat{S}^m$ for $m > 0$. Therefore,

$$
\hat{Z}^m_0 \hat{L}_{H_0} = \hat{L}_{H_0} \hat{Z}^m_0 = \hat{Z}^{m-1}_0 - \delta_1^m,
$$

$$
\hat{Z}^m_0 \hat{H}_0 = \hat{H}_0 \hat{S}^m_0.
$$
Here $\delta^m_0$ is the Kronecker delta. For $n \geq 1$ we have:

$$\dot{Z}_n^m L_{H_0} = \sum_{i=0}^{m} \dot{Z}_{n-1}^m L_i, \quad \dot{Z}_0^m L_{H_0} = \sum_{i=1}^{m} \dot{Z}_{n-1}^{m-i} L_i - \dot{Z}_{n-1}^m L_i = \dot{Z}_{n-1}^m - \dot{Z}_{n-1}^m L_i,$$

$$\dot{L}_{H_0} \dot{Z}_n^m = \sum_{i=0}^{m} \dot{L}_{H_0} \dot{Z}_i^1 L_{H_0} = \sum_{i=1}^{m} \dot{L}_i \dot{Z}_{n-1}^{m-i} - \dot{L}_i \dot{Z}_{n-1}^m = \dot{Z}_{n-1}^m - \dot{L}_i \dot{Z}_{n-1}^m.$$

$$\dot{Z}_n^m H_0 = \sum_{i=0}^{m} \dot{Z}_{n-1}^m L_i H_0 = \dot{Z}_{n-1}^m \dot{L}_i H_0 = -\dot{Z}_{n-1}^m H_i = -\dot{Z}_{n-1}^{m-1} H_i + \delta^m_1 \delta^m_1 H_i.$$

Next, we will use finite double-indexed operatorial sums

$$\hat{\mathcal{R}}_H^{(N)(k)} = -\sum_{n=0}^{N} \alpha^n \dot{Z}_{n}^{n+k},$$

(A.3)

having the following asymptotic behavior

$$\hat{\mathcal{R}}_H^{(N)(k)} = \begin{cases} \hat{S}^k + O(\alpha) & \text{if } k \geq 1, \\ -\hat{P} + O(\alpha) & \text{if } k = 0, \\ O(\alpha^k) & \text{if } k < 0. \end{cases}$$

These sums unify the expressions for

$$\hat{\mathcal{P}}_H^{(N)} = -\hat{\mathcal{R}}_H^{(N)(0)} \quad \hat{\mathcal{S}}_H^{(N)} = \hat{\mathcal{R}}_H^{(N)(1)} \quad \hat{\mathcal{D}}_H^{(N)} = -\hat{\mathcal{R}}_H^{(N)(-1)}.$$

Their actions on the perturbed Hamiltonian $H$ are as follows:

$$\hat{\mathcal{R}}_H^{(N)(k)} L_H = -\dot{Z}_0^k L_{H_0} - \sum_{n=1}^{N} \alpha^n \left( \dot{Z}_n^k L_{H_0} + \dot{Z}_{n-1}^{n+k-1} L_i \right) + O(\alpha^{N+1})$$

$$= \delta^k_1 + \hat{\mathcal{R}}_H^{(N)(k-1)} + O(\alpha^{N+1}),$$

$$\hat{L}_i \hat{\mathcal{R}}_H^{(N)(k)} = \ldots = \delta^k_1 + \hat{\mathcal{R}}_H^{(N)(k-1)} + O(\alpha^{N+1}),$$

(A.4)

$$\hat{\mathcal{R}}_H^{(N)(k)} H = -\dot{Z}_0^k H_0 - \sum_{n=1}^{N} \alpha^n \left( \dot{Z}_n^k H_0 + \dot{Z}_{n-1}^{n+k-1} H_i \right) + O(\alpha^{N+1}) = -\delta^k_1 H + O(\alpha^{N+1}).$$

Consider now the resolvent series truncated at $N^{th}$ order in $\alpha$ and $M^{th}$ order in $z$:

$$\mathcal{R}_H^{(N,M)}(z) = \sum_{k=-N}^{M+1} \hat{R}_H^{(N)(k)} z^{k-1} = -\sum_{k=-N-1}^{M} z^k \left( \sum_{n=0}^{N} \alpha^n \dot{Z}_n^{n+k+1} \right).$$

$\mathcal{R}_H^{(N,M)}(z)$ is an explicitly meromorphic function of complex $z$. We will use it like a generating function in probability theory. Powers of $z$ will serve as placeholders for simultaneous transformations of expressions. Due to the identities listed above,

$$\hat{\mathcal{R}}_H^{(N,M)}(z) L_H = \sum_{k=-N}^{M+1} z^{k-1} \hat{R}_H^{(N)(k)} L_H = 1 + z \hat{R}_H^{(N,M)}(z) - z^{M+1} \hat{R}_H^{(N)(M+1)} + O(\alpha^{N+1}),$$

$$\hat{L}_i \hat{R}_H^{(N,M)}(z) = 1 + z \hat{R}_H^{(N,M)}(z) - z^{M+1} \hat{R}_H^{(N)(M+1)} + O(\alpha^{N+1}).$$
Here, the term with $z^{M+1}$ represents the edge effect of truncation. Therefore the following expressions will approximate the identity operator

$$\mathcal{R}_H^{[N,M]}(z)(\mathbf{L}_H - z) + z^{M+1}\mathcal{R}_H^{[N,(M+1)]} = 1 + O(\alpha^{N+1}),$$

$$\mathbf{L}_H - z)\mathcal{R}_H^{[N,M]}(z) + z^{M+1}\mathcal{R}_H^{[N,(M+1)]} = 1 + O(\alpha^{N+1}).$$

Corresponding approximate Hilbert identity is as follows:

$$\mathcal{R}_H^{[N,M]}(z_1) - \mathcal{R}_H^{[N,M]}(z_2) = (z_1 - z_2)\mathcal{R}_H^{[N,M]}(z_1)\mathcal{R}_H^{[N,M]}(z_2)$$

$$- z_1^{M+1}\mathcal{R}_H^{[N,(M+1)]}\mathcal{R}_H^{[N,M]}(z_2) + z_2^{M+1}\mathcal{R}_H^{[N,M]}(z_1)\mathcal{R}_H^{[N,(M+1)]} + O(\alpha^{N+1}).$$

Similarly to (21) we can obtain the expression for the product of the two coefficients

$$\hat{R}_H^{[N](m)}\hat{R}_H^{[N](n)} = \left(\frac{1}{2\pi i}\right)^2 \oint_{|z_1|=\varepsilon_1} \oint_{|z_2|=\varepsilon_2} \mathcal{R}_H^{[N,M]}(z_1)\mathcal{R}_H^{[N,M]}(z_2) z_1^{-m} z_2^{-n} d\bar{z}_1 d\bar{z}_2$$

$$= (\eta_m + \eta_n - 1)\hat{R}_H^{[N](m+n)} - \eta_{m-M-1}\hat{R}_H^{[N](M+1)}\hat{R}_H^{[N](m-n-M-1)}$$

$$+ (1 - \eta_{m-M-1})\hat{R}_H^{[N](m-n-M-1)}\hat{R}_H^{[N](M+1)} + O(\alpha^{N+1})$$

For any $m$ and $n$ we can choose the truncation order $M$, so that $M \geq m + n + N$ and $\hat{R}_H^{[N](m+n-M-1)} = O(\alpha^{N+1})$. Therefore,

$$\hat{R}_H^{[N](m)}\hat{R}_H^{[N](n)} = (\eta_m + \eta_n - 1)\hat{R}_H^{[N](m+n)} + O(\alpha^{N+1}) \quad (A.5)$$

From (A.4) and the coefficients of powers of $z$ in the above identity, it follows that:

- The finite sum $\hat{P}_H^{[N]}$ is the approximate projector $\hat{P}_H^{[N]}\hat{P}_H^{[N]} = \hat{P}_H^{[N]} + O(\alpha^{N+1})$.
- The sums $\hat{P}_H^{[N]}, \hat{S}_H^{[N]}$ and $\hat{D}_H^{[N]}$ obey approximately the same identities as the corresponding perturbative operators:

$$\hat{P}_H^{[N]}\hat{S}_H^{[N]} = 0 + O(\alpha^{N+1}), \quad \hat{S}_H^{[N]}\hat{P}_H^{[N]} = 0 + O(\alpha^{N+1}),$$

$$\hat{D}_H^{[N]}\hat{S}_H^{[N]} = 0 + O(\alpha^{N+1}), \quad \hat{S}_H^{[N]}\hat{D}_H^{[N]} = 0 + O(\alpha^{N+1}),$$

$$\hat{P}_H^{[N]}\hat{D}_H^{[N]} = \hat{D}_H^{[N]} + O(\alpha^{N+1}), \quad \hat{D}_H^{[N]}\hat{P}_H^{[N]} = \hat{D}_H^{[N]} + O(\alpha^{N+1}).$$

- These operators act on the perturbed Hamiltonian $H = H_0 + \alpha H_i$ as follows:

$$\hat{P}_H^{[N]}H = H + O(\alpha^{N+1}),$$

$$\hat{S}_H^{[N]}H = 0 + O(\alpha^{N+1}), \quad \hat{D}_H^{[N]}H = 0 + O(\alpha^{N+1}),$$

- Interactions of Liouville operator with these sums are as follows:

$$\mathbf{L}_H\hat{P}_H^{[N]} = \hat{D}_H^{[N]} + O(\alpha^{N+1}), \quad \hat{P}_H^{[N]}\mathbf{L}_H = \hat{D}_H^{[N]} + O(\alpha^{N+1}),$$

$$\mathbf{S}_H^{[N]}\mathbf{L}_H = 1 - \hat{P}_H^{[N]} + O(\alpha^{N+1}), \quad \mathbf{L}_H\mathbf{S}_H^{[N]} = 1 - \hat{P}_H^{[N]} + O(\alpha^{N+1}),$$

$$\mathbf{L}_H\hat{D}_H^{[N]} = \left(\hat{D}_H^{[N]}\right)^2 + O(\alpha^{N+1}), \quad \hat{D}_H^{[N]}\mathbf{L}_H = \left(\hat{D}_H^{[N]}\right)^2 + O(\alpha^{N+1}).$$
Powers of $\hat{S}[^N_H]$ and $\hat{D}[^N_H]$ operators can be expressed as follows:

\[
\left( \hat{S}[^N_H] \right)^k = R[^{N}(k)] + O(\alpha^{N+1}) = -\sum_{n=0}^{N} \alpha^n \hat{Z}_n^{n+k} + O(\alpha^{N+1}),
\]

\[
\left( \hat{D}[^N_H] \right)^k = -R[^{N}(-k)] + O(\alpha^{N+1}) = \sum_{n=k}^{N} \alpha^n \hat{Z}_n^{n-k} + O(\alpha^{N+1}).
\]

See also the demo “perturbed operators” in the supplementary data files.

Appendix B. Canonical connection of the projectors.

Now we will use the truncated resolvent

\[
\hat{R}[^N_H](z) = \frac{1}{z} \hat{P}[^N_H] + \sum_{k=0}^{2N} z^k \left( \hat{S}[^N_H] \right)^{k+1} - \sum_{k=2}^{N+1} z^{-k} \left( \hat{D}[^N_H] \right)^{k-1} = -\sum_{k=-N-1}^{2N} z^k \left( \sum_{n=0}^{N} \alpha^n \hat{Z}_n^{n+k+1} \right),
\]

to prove the canonical connection of the perturbed and unperturbed projectors. In this section we set the order of truncation in $z$ to $2N$, as it was large enough to avoid edge effects originating from the expression

\[
\hat{R}[^N_H](z)(\hat{L}_H - z) + z^{2N+1} \left( \hat{S}[^N_H] \right)^{2N+1} = 1 + O(\alpha^{N+1}). \tag{B.1}
\]

In particular, because $\left( \hat{D}[^N_H] \right)^m = O(\alpha^m)$ and $\hat{S}[^N_H] \hat{D}[^N_H] = O(\alpha^{N+1})$, then for all integer $1 \leq k \leq N$ we have:

\[
\text{Res}_{z=0} \left( z^{2N+1} \left( \hat{R}[^N_H](z) \right)^k \right) = O(\alpha^{N+1}). \tag{B.2}
\]

Also, for any integer $k \geq 2$:

\[
\text{Res}_{z=0} \left( \left( \hat{R}[^N_H](z) \right)^k \right) = O(\alpha^{N+1}).
\]

As expected, the derivative of projector can be related to the residue:

\[
\text{Res}_{z=0} \left( \hat{R}[^N_H](z) \hat{L}_H \hat{R}[^N_H](z) \right) = \sum_{k=-N-1}^{N} \sum_{n=0}^{N} \sum_{m=0}^{N} \alpha^{n+m} \hat{Z}_n^{n+k+1} \hat{L}_H \hat{Z}_m^{m-k} = \sum_{k=0}^{N} (k+1) \alpha^k \hat{Z}_k^{k+1} + O(\alpha^{N+1}) = \left( \frac{\partial}{\partial \alpha} \hat{P}_H \right)^{[N]} + O(\alpha^{N+1}).
\]

There was no loss of accuracy, since we truncated the series after the differentiation.

Now we can construct the finite analogue of canonical resolvent identity \((27)\). The application of almost identity operator \((B.1)\) to Poisson bracket $[\hat{R}[^N_H](z_2)H_1, \hat{R}[^N_H](z)G]$
results in

\[
\begin{align*}
\mathcal{R}^N_H(z)\hat{L}^N_H & = \hat{L}^N_H \mathcal{R}^N_H(z) - \mathcal{R}^N_H(z)\hat{L}^N_H + z^{2N+1} \left( \left( \mathcal{S}^N_H \right)^{2N+1} \partial_{\alpha}N_{\hat{L}^N_H} - z^2 \mathcal{R}^N_H(z) \hat{L}^N_H \mathcal{R}^N_H(z) \right) \\
& + z^{2N+1} \left( \left( \mathcal{S}^N_H \right)^{2N+1} \hat{R}^N_H(z) \right) + O(\alpha^{N+1}).
\end{align*}
\]

We are interested in the residue of the above formula at \( z = 0 \):

\[
\left( \frac{\partial}{\partial \alpha} \hat{P}^N_H \right)^{[N]} = \hat{P}^N_H \mathcal{R}^N_H(z) - \mathcal{R}^N_H(z)\hat{P}^N_H + z^2 \text{Res}_{z=0} \left( \mathcal{R}^N_H(z)\hat{L}^N_H \mathcal{R}^N_H(z) \right) + z^{2N+1} \left( \left( \mathcal{S}^N_H \right)^{2N+1} \hat{R}^N_H(z) \right) + O(\alpha^{N+1}).
\]

We will show that the last residue is \( O(\alpha^{N+1}) \) also. The coefficient of \( z_2^{-1} \) in (B.3) is

\[
0 = \mathcal{R}^N_H(z)\hat{L}^N_{p^H} - \hat{L}^N_{p^H} \mathcal{R}^N_H(z) + R_{\mathcal{R}^N_H(z)} \hat{L}^N_{D^H} \mathcal{R}^N_H(z)
+ z^{2N+1} \left( \left( \mathcal{S}^N_H \right)^{2N+1} \hat{L}^N_{p^H} \mathcal{R}^N_H(z) - \mathcal{R}^N_H(z)\hat{L}^N_{p^H} \left( \mathcal{S}^N_H \right)^{2N+1} \right) + O(\alpha^{N+1}).
\]

Therefore,

\[
\text{Res}_{z=0} \left( \mathcal{R}^N_H(z)\hat{L}^N_{p^H} \mathcal{R}^N_H(z) \right) = \text{Res}_{z=0} \left( \mathcal{L}^N_{p^H} \mathcal{R}^N_H(z) \mathcal{R}^N_H(z) \right) - \text{Res}_{z=0} \left( \mathcal{R}^N_H(z)\hat{L}^N_{D^H} \mathcal{R}^N_H(z) \right) + O(\alpha^{N+1})
\]

\[
= -\text{Res}_{z=0} \left( \mathcal{R}^N_H(z)\hat{L}^N_{D^H} \mathcal{R}^N_H(z) \right) + O(\alpha^{N+1}).
\]

We can continue this process using coefficients of \( z_2^{-2} \), \( z_2^{-3} \), \ldots in (B.3)

\[
\text{Res}_{z=0} \left( \mathcal{R}^N_H(z)\hat{L}^N_{D^H} \mathcal{R}^N_H(z) \right) = -\text{Res}_{z=0} \left( \mathcal{R}^N_H(z)^2 \hat{L}^N_{D^H} \mathcal{R}^N_H(z) \right) + O(\alpha^{N+1})
\]

\[
\ldots = (-1)^{N+1} \text{Res}_{z=0} \left( \mathcal{R}^N_H(z)^{N+1} \hat{L}^N_{D^H} \mathcal{R}^N_H(z) \right) + O(\alpha^{N+1}) = O(\alpha^{N+1}).
\]

Inserting this into (B.4) concludes the proof that the projector canonically transforms

\[
\left( \frac{\partial}{\partial \alpha} \hat{P}^N_H \right)^{[N]} = \hat{L}^N_{S^N_H} \hat{P}^N_H - \hat{P}^N_H \hat{L}^N_{S^N_H} + O(\alpha^{N+1}),
\]

with the generator \( G^{[N]} = -S^N_H H_i \) in any perturbation order.
Appendix C. The square algorithm.

Relation (A.2) leads to an efficient computational algorithm for the generator $G^N = -\hat{S}_H^N H_i$. Consider a square table:

$$
\begin{array}{llllll}
F_0^0(x) & F_1^0(x) & F_2^0(x) & \ldots & F_0^{N+1}(x) \\
F_0^1(x) & F_1^1(x) & F_2^1(x) & \ldots & F_1^{N+1}(x) \\
& \ldots & \ldots & \ldots & \ldots \\
F_{N-1}^0(x) & F_{N-1}^1(x) & F_{N-1}^2(x) & \ldots & F_{N-1}^{N+1}(x) \\
& & F_N^{N+1}(x)
\end{array}
$$

Here the first row is as follows:

$$
F_0^0(x) = \hat{Z}_0^0 H_i = P H_i, \quad F_0^m(x) = \hat{Z}_0^m H_i = -\hat{S}_i^m H_i,
$$

and each next row is generated from the previous one according to the rule

$$
F_{n+1}^m(x) = \sum_{i=0}^{m} \hat{Z}_0^{m-i} L_i H_i F_n^i(x).
$$

The normalizing generator is given by $G^N = \sum_{n=0}^{N} a^n F_n^{n+1}(x)$. Obvious computational optimization is to store the quantities $L_i H_i F_n^i(x)$.

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